A Critique of Mathematical Errors in Gaussian Processes for Machine Learning

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Abstract

This article critiques the statement in Rasmussen and Williams' book *Gaussian Processes* for Machine Learning that "the eigenfunctions of stationary kernels are Fourier basis functions." This claim is fundamentally flawed, both categorically and factually. The critique identifies the errors and provides the correct mathematical understanding.

1 Introduction

The book Gaussian Processes for Machine Learning by Rasmussen and Williams is widely cited in the field of machine learning. However, it contains a significant mathematical error in its characterization of eigenfunctions of stationary kernels. Specifically, the statement that "the eigenfunctions of stationary kernels are Fourier basis functions" is incorrect. This critique highlights the errors in this claim and clarifies the correct mathematical formulation.

2 The Errors in Detail

2.1 Category Error: Kernels vs. Operators

The first error lies in the attribution of eigenfunctions to kernels themselves. In functional analysis, eigenfunctions are associated with operators, not kernels. A kernel function k(x, y) defines an integral operator A on a function space as:

$$(Af)(x) = \int k(x, y) f(y) dy$$

$$\tag{1}$$

The eigenvalue problem for A is:

$$A \phi = \lambda \phi \tag{2}$$

where ϕ is the eigenfunction and λ is the eigenvalue. The statement in question fundamentally confuses these mathematical objects.

2.2 Factual Error: Incorrect Characterization of Eigenfunctions

The second error is the claim that the eigenfunctions of stationary kernels are Fourier basis functions. This is demonstrably false. While Fourier basis functions are eigenfunctions of the translation operator, they are not generally eigenfunctions of integral operators defined by stationary kernels.

For example, consider the Gaussian kernel:

$$k(x,y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right)$$
 (3)

The eigenfunctions of the integral operator defined by this kernel are related to Hermite polynomials modulated by a Gaussian envelope:

$$\phi_n(x) = H_n(x) e^{-x^2} \tag{4}$$

where H_n are Hermite polynomials. These eigenfunctions form an orthogonal basis for the function space and are clearly not Fourier basis functions.

This counterexample demonstrates that the general claim about Fourier basis functions being eigenfunctions of all stationary kernels is false.

3 Conclusion

The statement that "the eigenfunctions of stationary kernels are Fourier basis functions" is mathematically incorrect on multiple levels. It represents a fundamental misunderstanding of functional analysis principles. The correct approach requires distinguishing between kernels and operators and recognizing that eigenfunctions depend on the specific form of the kernel.

This critique highlights the need for greater mathematical rigor in foundational texts to prevent such errors from propagating through related fields.