Additive Structure, Product Kernel, and Unital Gaussian Process

Shaowei Cheng
Institute of Statistics, National Tsing Hua University, Taiwan

Abstract

The utilization of product kernels in Gaussian processes has gained substantial popularity due to their efficiency in capturing complex dependencies between factors and response while maintaining a minimal number of parameters. However, the performance of product kernels would degrade when data exhibits certain additive structures. In this work, we provide a detailed demonstration of this limitation through illustrative examples. On the other hand, although additive kernels offer an alternative for addressing additive structures, they may lead to a significant increase in the number of parameters when dealing with interactions. In response to this issue, we propose unital Gaussian process (GP). It partitions the factors into distinct groups, where the structure between groups adheres to a "unital structure", while within each group, a product kernel structure is maintained. This unique design allows the unital GP to accommodate additive structures while keeping the number of parameters at a reasonable level. A derivation is provided to explain how the unital GP can converge to a kernel with an additive structure or a product kernel as the parameters vary in different ways. We show the superior performance of the unital GP in the presence of additive structures through examples. Finally, we discuss the insights and challenges related to local smoothing introduced by the unital GP. This work is a collaborative effort with Dr. Chih-Li Sung at Michigan State University.