Necessary condition for matrix-valued kernels

Miaoyan Wang, April 26, 2020

Theorem 0.1 (Necessary condition). Suppose $K: \mathbb{R}^{d' \times d} \times \mathbb{R}^{d' \times d} \mapsto \mathbb{R}^{d \times d}$ is a function that takes as input a pair of matrices and produces a matrix. Let $\{X_i \in \mathbb{R}^{d' \times d} : i \in [n]\}$ denote a set of input matrices, and let K denote an order-4 (d, d, n, n)-dimensional array,

$$\mathcal{K} = [\![\mathcal{K}(i, i', p, p')]\!], \text{ where } \mathcal{K}(i, i', p, p') \text{ is the } (p, p')\text{-th entry of the matrix } \mathbf{K}(\mathbf{X}_i, \mathbf{X}_{i'}).$$

Then, the factorization $K(X, X') = h(X)^T h(X')$ exists for some mapping h, only if both of the following conditions hold:

- (1) For every index $i \in [n]$, the slice $K(i, i, \cdot, \cdot) \in \mathbb{R}^{d \times d}$ is a symmetric, positive definite matrix.
- (2) For every index $p \in [d]$, the slice $\mathcal{K}(\cdot, \cdot, p, p) \in \mathbb{R}^{n \times n}$ is a symmetric, positive definite matrix.