How to Normalize a Kernel Matrix

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Abstract

We describe how to normalize a kernel matrix.

Let $K \in \mathbb{R}^{n \times n}$ be a kernel matrix. K is normalized iff $K_{ii} = 1 \; \forall i \in \{1, \ldots, n\}$. We presume that $K = XX^T$ for some $X \in \mathbb{R}^{n \times d}$. Define X_i to be the i^{th} row of X. Note $K_{ii} = 1 \iff X_i X_i^T = 1$. Define $\tilde{X}$ to be a row-normalized version of X. That is, $\tilde{X}_i = X_i / \sqrt{X_i X_i^T}$. Let $\tilde{K} = \tilde{X}\tilde{X}^T$. Note that $\tilde{K}_{ii} = 1 \; \forall i$.

Now, given an unnormalized kernel matrix, K, we would like to normalize it; i.e. we would like to construct $\tilde{K}$. Note that $\tilde{K}_{ij} = K_{ij} / \sqrt{K_{ii} K_{jj}}$. Define $\vec{k} = (1/\sqrt{K_{11}}, \ldots, 1/\sqrt{K_{nn}})$. Then, $\tilde{K} = K * (\vec{k}\vec{k}^T)$, where $*$ denotes element-wise product.