

We give a proof of the positive definiteness of convolution kernels. Convolution kernels (Haussler '99) are defined by

$$K(x, y) = \sum_{\vec{x} \in R^{-1}(x)} \sum_{\vec{y} \in R^{-1}(y)} k(\vec{x}, \vec{y}). \quad (1)$$

Here $\vec{x}, \vec{y} \in X$ are considered as parts of x and y ; $k(\vec{x}, \vec{y})$ is a positive definite kernel defined on $X \times X$; R is a relation which associates a *finite* subset of X with each x in the object space \mathcal{X} , and this subset is denoted by $R^{-1}(x)$.

To simplify notation, let us write $R^{-1}(x)$ as A_x . Thus $K(x, y)$ assigns a number to two finite subsets $A_x, A_y \subseteq X$. We can *extend* this definition to all pairs of finite subsets of X by defining a kernel $K^s : \mathcal{U} \times \mathcal{U} \rightarrow \mathfrak{R}$, where $\mathcal{U} = \{A \mid A \text{ finite}, A \subseteq X\}$,

$$K^s(A, B) = \sum_{\vec{x} \in A} \sum_{\vec{y} \in B} k(\vec{x}, \vec{y}).$$

Clearly, if the extension K^s is a positive definite kernel, then K is positive definite.

We shall prove this using the random variable “trick.” For any vector-valued random variable Y , taking values in \mathfrak{R}^n , the matrix $E\{YY^\top\}$ is clearly always positive definite, because $c^\top E\{YY^\top\}c = E\{(c^\top Y)^2\} \geq 0$ for any vector $c \in \mathfrak{R}^n$.

Lemma 1. *K^s is positive definite.*

Proof. We need to show for any n , $A_1, \dots, A_n \subseteq X$, the matrix \bar{K} with $\bar{K}_{ij} = K^s(A_i, A_j)$ is positive definite. We shall prove this by constructing an n -dimensional random variable $Y = (Y_1, \dots, Y_n)^\top$, taking values in \mathfrak{R}^n , such that $E\{YY^\top\} = \bar{K}$. Let $A = \cup_{i=1}^n A_i$ and m be the size of A . Create an m -dimensional zero-mean Gaussian random variable Z , whose components are indexed by $a \in A$ and whose covariance is defined by

$$E\{Z_a Z_{\hat{a}}\} = k(a, \hat{a}), \quad a, \hat{a} \in A.$$

We now define $Y_i, i = 1, \dots, n$ by

$$Y_i = \sum_{a \in A_i} Z_a.$$

Then,

$$E\{Y_i Y_j\} = E\left\{\left(\sum_{a \in A_i} Z_a\right)\left(\sum_{\hat{a} \in A_j} Z_{\hat{a}}\right)\right\} = \sum_{a \in A_i} \sum_{\hat{a} \in A_j} E\{Z_a Z_{\hat{a}}\} = \sum_{a \in A_i} \sum_{\hat{a} \in A_j} k(a, \hat{a}) = K^s(A_i, A_j),$$

so $E\{YY^\top\} = \bar{K}$; this completes our proof. \square