Jaccard Index is a Kernel **Huitao Shen** Huitao Shen Huitao Shen Huitao Shen Huitao Shen Huitao Shen Huitao Shen

Proposition 1. *Jaccard index defined for two finite nonempty sets* A*,* B *in a universe* Ω *with finite elements is a kernel:*

$$
J(A,B) = \frac{|A \cap B|}{|A \cup B|}.\tag{1}
$$

Proof. We need several preliminary results in order to prove the above proposition.

Lemma 2. *Closure properties of kernels:*

- If k_1 and k_2 are kernels, then so is $ak_1 + bk_2$ for scalars $a, b \ge 0$.
- *If* k_1 *and* k_2 *are kernels, then so is* k_1k_2 *.*

See lecture note for a proof.

Lemma 3. *If* $k(x, y)$ *is a kernel bounded from above:* $\max_{x, y} k(x, y) = \max_{x} k(x, x) < D < \infty$ *, then*

$$
k'(x, y) = \frac{1}{D - k(x, y)},
$$
\n(2)

is also a kernel.

Proof. Using series expansion:

$$
k'(x,y) = \frac{1}{D} \sum_{n=0}^{\infty} \left(\frac{k(x,y)}{D} \right)^n.
$$
 (3)

The expansion converges because $\max_{x,y} k(x,y) < D$. With Lemma [2,](#page-0-0) $k'(x,y)$ is a kernel. (One might wonder whether Lemma [2](#page-0-0) works for countable infinite many terms. The answer is positive as long as the series converges, because essentially we only need to prove the positive semi-definiteness of the kernel.) \Box

One last result we need is

Lemma 4. For two nonempty sets A, B with finite elements, $k(A, B) = |A \cap B|$ and $k(A, B) = |\overline{A} \cap \overline{B}|$ are kernels.

Proof. Use bit encoding of the set. For $k(A, B) = |A \cap B|$, explicitly construct feature map $\phi(A)$ as follows: $\phi(A)$ is a vector such that $[\phi(A)]_i = 1$ if i-th element is in A and $[\phi(A)]_i = 0$ otherwise. Then $k(A, B) = \phi(A)^T \phi(B)$. For $k(A, B) = |\bar{A} \cap \bar{B}|$, use $\psi = 1 - \phi$ as the feature map. \Box

Note $A \cup B = \overline{A \cap B}$, where $\overline{A} = \Omega - A$ is the complement of set A. It follows $|A \cup B| = |\Omega| - |\overline{A} \cap \overline{B}|$. Using Lemma [3](#page-0-1) and [4,](#page-0-2) $1/|A \cup B|$ is a kernel. Then using Lemma [2](#page-0-0) again, $|A \cap B|/|A \cup B|$ is a kernel. \Box

Remark. What is the feature map of the Jaccard index? It should be very hard to write down explicitly. Let us take a step back and consider the feature map of $k(A, B) = 1/|A \cup B|$, which is also proved to be a kernel:

$$
k(A,B) = \frac{1}{|A \cup B|} = \frac{1}{|\Omega| - |\bar{A} \cap \bar{B}|} = \frac{1}{|\Omega|} \sum_{n=0}^{\infty} \left(\frac{|\bar{A} \cap \bar{B}|}{|\Omega|} \right)^n.
$$
 (4)

Since we already know the feature map of $|\bar{A} \cap \bar{B}|$ as ψ , the feature map of $|\bar{A} \cap \bar{B}|^n$ can simply be the tensor product $\psi^{\otimes n}$ in a $|\Omega|n$ -dimensional space. Because the infinite summation is involved, the feature mapping of $1/|A \cup B|$ is also in a countable infinite dimensional space:

$$
\varphi = \frac{1}{\sqrt{|\Omega|}} \sum_{n=0}^{\infty} \frac{\psi^{\otimes n}}{\sqrt{|\Omega|^n}},\tag{5}
$$

where the summation is the direct sum.

With the feature map of $|A \cap B|$: ϕ (finite-dimensional) and $1/|A \cup B|$: φ (infinite-dimensional), the feature map of Jaccard index can be constructed similarly using tensor product: $\phi \otimes \varphi$ and is infinite-dimensional. Note that this construction does not necessarily exclude a finite-dimensional feature map because feature map is not unique.

Proposition 5. *Jaccard index defined for two finite nonempty sets* A*,* B *in a universe* Ω *with infinite elements is a kernel:*

$$
J(A,B) = \frac{|A \cap B|}{|A \cup B|}.\tag{6}
$$

Proof. Now since $\max_x k(x, x) = |\Omega| = \infty$, we cannot use Lemma [3.](#page-0-1) The work around is to use another representation of $|A \cup B|$ and the following lemma:

Lemma 6. *The following index for two nonempty sets* A, B *is a kernel:*

$$
H(A, B) = \frac{1}{|A| + |B|}.
$$
\n(7)

Proof. According to Mercer's theorem, we need to prove its positive semi-definiteness. In particular, it suffices to prove any $n \times n$ matrix M, where $n \in \mathbb{N}$ and $M_{i,j} = 1/(i+j)$ is positive semi-definite. This is exactly a Hilbert matrix and its positive semi-definiteness is well-known. To prove this fact, for all c_i , c_j :

$$
\sum_{i,j=1}^{n} c_i M_{i,j} c_j = \sum_{i,j=1}^{n} \frac{c_i c_j}{i+j} = \sum_{i,j=1}^{n} c_i c_j \int_0^1 t^{i+j-1} dt = \int_0^1 t \left(\sum_{i=1}^{n} c_i t^{i-1}\right)^2 dt \ge 0.
$$
 (8)

Hence we have proved $H(A, B)$ is a kernel. Note that one can also use another trick $1/(i + j) = \int_0^{+\infty} e^{-(i+j)t} dt$ in the proof. \Box

Decompose $|A \cup B|$ as

$$
\frac{1}{|A \cup B|} = \frac{1}{|A| + |B| - |A \cap B|} = \frac{1}{|A| + |B|} \frac{1}{1 - \frac{|A \cap B|}{|A| + |B|}} = \frac{H(A, B)}{1 - H(A, B)|A \cap B|}. \tag{9}
$$

Using Lemma [2,](#page-0-0) [3,](#page-0-1) [4](#page-0-2) and [6,](#page-1-0) $1/|A \cup B|$ is a kernel even if the universe Ω has infinite elements. Then use Lemma [2](#page-0-0) again, $J(A, B)$ is a kernel. \Box