## Jaccard Index is a Kernel

## Huitao Shen

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

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

$$k'(x,y) = \frac{1}{D - k(x,y)},$$
(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, k'(x,y) is a kernel. (One might wonder whether Lemma 2 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.)

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  $k(A, B) = |\overline{A} \cap \overline{B}|$ , use  $\psi = 1 - \phi$  as the feature map.

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

*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  $\psi$ , 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  $|A \cap B|$ :  $\phi$  (finite-dimensional) and  $1/|A \cup B|$ :  $\varphi$  (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  $\Omega$  with infinite elements is a kernel:

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

*Proof.* Now since  $\max_x k(x, x) = |\Omega| = \infty$ , we cannot use Lemma 3. 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:

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

Decompose  $|A \cup B|$  as

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

Using Lemma 2, 3, 4 and 6,  $1/|A \cup B|$  is a kernel even if the universe  $\Omega$  has infinite elements. Then use Lemma 2 again, J(A, B) is a kernel.