Kernels for cross-species clustering

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1 Mathematics

Suppose K_1 and K_2 denote kernel matrices computed on n_1 and n_2 objects from two separate species of objects respectively. Further suppose that an n_1 by n_2 matrix T exists which maps objects from one set to another. Then define the cross-species kernel $\mathcal{K}$ as

$$\mathcal{K} = \begin{bmatrix} K_1 K_1 & K_1 T K_2 \\ K_2' T' K_1' & K_2 K_2 \end{bmatrix}$$

where A' denotes the transpose of a matrix A. The blocks along the diagonal represent the within-species product while the off-diagonal blocks represent a transformation of objects from one species into the kernel space of the other. Note that the matrices K could also be replaced with $\sqrt{K}$ for better matrix conditioning.

In order for $\mathcal{K}$ to be a valid kernel, it must be positive semidefinite which means that for any value x_1 and x_2,

$$[x_1' \; x_2'] \begin{bmatrix} K_1 K_1 & K_1 T K_2 \\ K_2' T' K_1' & K_2 K_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \geq 0.$$

Multiplying the right vector yields

$$[x_1' \; x_2'] \begin{bmatrix} K_1 K_1 x_1 + K_1 T K_2 x_2 \\ K_2' T' K_1' x_1 + K_2 K_2 x_2 \end{bmatrix}.$$

Now multiplying by the left vector and using the fact that a symmetric matrix is equal to its transpose yields

$$\begin{aligned} &x_1' K_1' K_1 x_1 + x_1' K_1' T K_2 x_2 + \\ &x_2' K_2' T' K_1 x_1 + x_2' K_2' K_2 x_2. \end{aligned}$$

Combining like terms and using the fact that $A'B' = (BA)'$ for symmetric matrices A and B produces

$$(K_1x_1)'(K_1x_1) + (K_1x_1)'T(K_2x_2) + \\ (K_2x_2)'T'(K_1x_1) + (K_2x_2)'(K_2x_2).$$

Using algebraic manipulations, the above is equivalent to

$$[(K_1x_1)' \ (K_2x_2)'] \begin{bmatrix} I & T \\ T & I \end{bmatrix} \begin{bmatrix} (K_1x_1) \\ (K_2x_2) \end{bmatrix}$$

which is ≥ 0 if the central matrix involving the identity matrix I and the mapping matrix T is positive semidefinite. Note that proving this imposes a much stronger condition than required for the current purposes since (K_1x_1) and (K_2x_2) may not span all of the space of the central matrix. If $T == I$ such that each object of one space maps uniquely to an object of the other space, then the condition for positive semidefiniteness holds; in fact, all eigenvalues are equal to 2. In general, the condition is valid when T itself is positive semidefinite.