Kernel Methods for Radial Transformed Compositional Data with Many Zeros,

Compositional data analysis with a high proportion of zeros has gained increasing popularity, especially in chemometrics and human gut microbiomes research. Statistical analyses of this type of data are typically carried out via a log-ratio transformation after replacing zeros with small positive values. We should note, however, that this procedure is geometrically improper, as it causes anomalous distortions through the transformation. We propose a radial transformation that does not require zero substitutions and more importantly results in essential equivalence between domains before and after the transformation. We show that a rich class of kernels on hyperspheres can successfully define a kernel embedding for compositional data based on this equivalence. The applicability of the proposed approach is demonstrated with kernel principal component analysis.

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