

VALISE: A ROBUST VERTEX HUNTING ALGORITHM

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Abstract: Given data vectors $X_1, \dots, X_n \in \mathbb{R}^r$, where X_i is a noisy observation of X_i^* , and X_1^*, \dots, X_n^* are contained in an unknown simplex with K vertices, vertex hunting (VH) is the problem of estimating the vertices of the true simplex. VH is a building block of several algorithms in hyperspectral remote sensing, soft clustering, topic modeling, and network mixed membership estimation. The popular VH algorithms are susceptible to outliers, whose estimation errors are governed by $\max_i \|X_i - X_i^*\|$. We propose a robust VH algorithm that properly shrinks estimated vertices towards the interior of data cloud, so as to mitigate the effect of outliers. The level of shrinkage is determined by maximizing a pseudo likelihood and has no tuning parameter. We show that, when the barycentric coordinates of X_1^*, \dots, X_n^* come from a Dirichlet distribution, the proposed method has a faster rate of convergence than several popular VH algorithms.

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1. Introduction

Let $\mathcal{S} \subset \mathbb{R}^r$ be a K -vertex simplex, whose vertices are denoted by V_1, V_2, \dots, V_K . Suppose $X_1^*, X_2^*, \dots, X_n^*$ are non-stochastic vectors in this simplex. Equivalently, each X_i^* is a convex combination of the vertices:

$$X_i^* = \sum_{k=1}^K \pi_i(k) V_k, \quad 1 \leq i \leq n. \quad (1.1)$$

Here $\pi_i = \{\pi_i(1), \dots, \pi_i(K)\}' \in \mathbb{R}_+^K$ is a vector in the standard simplex such that $0 \leq \pi_i(k) \leq 1$ for $0 \leq k \leq K$ and $\sum_{k=1}^K \pi_i(k) = 1$. The entries of π_i are called the barycentric coordinates of X_i^* . We call an algorithm a Vertex Hunting (VH) algorithm if it does the following job: Given input $X_1, X_2, \dots, X_n \in \mathbb{R}^r$, where each X_i is a noisy observation of X_i^* , the algorithm outputs the estimated vertices $\hat{V}_1, \hat{V}_2, \dots, \hat{V}_K$.

Vertex hunting has a lot of applications in hyperspectral unmixing (Bioucas-Dias et al., 2012). A hyperspectral image is a mixture of signals from different pure materials, and vertex hunting algorithms are used to find the spectral signature of each pure material. Another application of vertex hunting is

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