Fast Initialization

Yangrui Liu[†]

July 23, 2023

1 Notation

- $\text{conv}(\mathcal{S})$ denotes the convex hull of the set $\mathcal{S}$ [1].
- $\mathbb{R}^N$ is the N-dimensional Euclidean space.
- $\mathbb{R}^{M\times N}$ is the $(M \times N)$-dimensional real-valued matrix space.
- $\mathbf{0}$ is the all-zero vector/matrix/tensor with dimensionality specified in its subscript.
- $\mathbf{1}$ is the all-one vector/matrix/tensor with dimensionality specified in its subscript.
- $\boldsymbol{M}^T$ is the transpose of the matrix $\boldsymbol{M}$, and $\boldsymbol{M}^{-1}$ is the inverse of the matrix $\boldsymbol{M}$.
- $\|\cdot\|_2$ denotes ℓ_2-norm.

2 Related Background

A p-dimensional ellipsoid in $\mathbb{R}^n$ can be written as an "affine mapping" of the Euclidean unit ball:

$$\mathcal{E}(\boldsymbol{F}, \boldsymbol{c}) = \{\boldsymbol{F}\boldsymbol{x} + \boldsymbol{c} | \boldsymbol{x} \in B\}, \tag{1}$$

where $B = \{\boldsymbol{x} | \|\boldsymbol{x}\|_2 \leq 1\}$ is the Euclidean unit ball, $\boldsymbol{c}$ is the center of the ellipsoid, and $\boldsymbol{F}$ is the John ellipsoid matrix of full column rank. We can also simply represent the ellipsoid as:

$$\mathcal{E}(\boldsymbol{F}, \boldsymbol{c}) = \boldsymbol{F}B + \boldsymbol{c}. \tag{2}$$

John ellipsoid is defined as the maximum-volume ellipsoid inscribed in the data convex hull.

3 Closed-Form Solution for the John Ellipsoid of a Fixed Simplex

In this section, we derive the closed-form solution for the John ellipsoid of a fixed simplex, aiming to find the John ellipsoid matrix $\boldsymbol{F}$ and center $\boldsymbol{c}$ that define the shape and position of the John ellipsoid. This derivation is based on the specific problem of fast initialization of the John ellipsoid, which involves computing the matrix $\boldsymbol{F}$ and vector $\boldsymbol{c}$ of the John ellipsoid of the simplex obtained from the successive projections algorithm (SPA) [2]. This initialization can be utilized as a starting point for the subsequent calculation of the maximum inscribed ellipsoid within the data convex hull. Given a hyperspectral image, we employ SPA to obtain a dimension-reduced signature matrix

[†]Department of Electrical Engineering, Tainan, Taiwan (R.O.C.) E-mail: `q36083030@gs.ncku.edu.tw`; Website: `https://sites.google.com/view/chiahsianglin/home`

$\boldsymbol{M}_0 = [\boldsymbol{m}_1, \ldots, \boldsymbol{m}_p] \in \mathbb{R}^{n\times p}$, where p is the number of endmembers and $n = p - 1$. Since the vectors $\{\boldsymbol{m}_1, \ldots, \boldsymbol{m}_p\}$ are affinely independent, they form a simplex $\mathrm{conv}\{\boldsymbol{m}_1, \ldots, \boldsymbol{m}_p\}$.

Our primary objective is to compute the John ellipsoid matrix $\boldsymbol{F}$ based on establishing the relationship between simplex $\mathrm{conv}\{\boldsymbol{m}_1, \ldots, \boldsymbol{m}_p\}$ and the simplex whose John ellipsoid is the unit ellipsoid.

3.1 Constructing a Simplex with a Unit Ball as its John Ellipsoid

In order to construct the simplex whose John ellipsoid is unit ball B, we start by operating on the identity matrix $\boldsymbol{E} = [\boldsymbol{e}_1, \ldots, \boldsymbol{e}_p] \in \mathbb{R}^{p\times p}$, where $\boldsymbol{e}_i$ denotes a unit vector and $\mathrm{conv}\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_p\}$ is a unit simplex. To center the unit simplex, we subtract the mean vector $\boldsymbol{d}$ from each column of $\boldsymbol{E}$, resulting in a new centered identity matrix denoted as $\bar{\boldsymbol{E}} = \boldsymbol{E} - \boldsymbol{d}\boldsymbol{1}_p^T \in \mathbb{R}^{p\times p}$.

Next, we apply principal component analysis (PCA) [3] on the $\bar{\boldsymbol{E}}$ to perform dimensionality reduction. This process yields the matrix $\hat{\boldsymbol{B}} = [\hat{\boldsymbol{b}}_1, \ldots, \hat{\boldsymbol{b}}_p] \in \mathbb{R}^{n\times p}$, whose columns forms a regular simplex $\mathrm{conv}\{\hat{\boldsymbol{b}}_1, \ldots, \hat{\boldsymbol{b}}_p\}$. Therefore, the simplex $\mathrm{conv}\{\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p\}$ whose John ellipsoid is the unit ball can be obtained by scaling the simplex $\mathrm{conv}\{\hat{\boldsymbol{b}}_1, \ldots, \hat{\boldsymbol{b}}_p\}$ with a scaled factor r, given by the equation:

$$\boldsymbol{B} = \frac{\hat{\boldsymbol{B}}}{r}, \tag{3}$$

where $\boldsymbol{B} = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p] \in \mathbb{R}^{n\times p}$. The scaling factor r is computed using the formula:

$$r = \left\| \frac{\boldsymbol{1}p}{p} - \frac{\boldsymbol{1}p}{n} \right\|_2 \tag{4}$$

This scaling factor ensures that the unit ball B is derived appropriately from the centered simplex $\bar{\boldsymbol{E}}$.

3.2 Closed-Form Solution of $\boldsymbol{F}$ and $\boldsymbol{c}$

After obtaining the simplex $\mathrm{conv}\{\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p\}$ with the unit ball as its John ellipsoid, our goal is to establish a relationship between $\boldsymbol{B}$ and the signature matrix $\boldsymbol{M}_0$.

Let $\mathcal{E}(\boldsymbol{F}, \boldsymbol{c})$ be the John ellipsoid of the simplex $\mathrm{conv}\{\boldsymbol{m}_1, \ldots, \boldsymbol{m}_p\}$, and $\mathcal{E}(\boldsymbol{G}, \boldsymbol{d})$ be the John ellipsoid of the convex hull of the simplex $\mathrm{conv}\{\boldsymbol{b}_1, \ldots, \boldsymbol{b}_p\}$. Mathematically, these two ellipsoids can be expressed as $\mathcal{E}(\boldsymbol{F}, \boldsymbol{c}) = \boldsymbol{F}B + \boldsymbol{c}$ and $\mathcal{E}(\boldsymbol{G}, \boldsymbol{d}) = \boldsymbol{G}B + \boldsymbol{d}$. Thus, we establish the mathematical relationship between $\boldsymbol{B}$ and $\boldsymbol{M}_0$ by :

$$\boldsymbol{G}^{-1}(\boldsymbol{B} - \boldsymbol{d}\boldsymbol{1}_p^T) = \boldsymbol{F}^{-1}(\boldsymbol{M}_0 - \boldsymbol{c}\boldsymbol{1}_p^T), \tag{5}$$

where $\boldsymbol{c}$ is the center of the convex hull $\mathrm{conv}\{\boldsymbol{m}_1, \ldots, \boldsymbol{m}_p\}$. Therefore, the closed-form solution of $\boldsymbol{c}$ can be computed as:

$$\boldsymbol{c} = \frac{1}{p} \sum_{i=1}^{p} \sqrt{\boldsymbol{m}_i} \tag{6}$$

As the John ellipsoid of the convex hull of matrix $\boldsymbol{B}$ is the unit ellipsoid, it follows that the matrices $\boldsymbol{G}$ and vector $\boldsymbol{d}$ correspond to the identity matrix $\boldsymbol{I}_n$ and the zero vector $\boldsymbol{0}_n$, respectively. Therefore, the John ellipsoid matrix $\boldsymbol{F}$ of the convex hull of $\boldsymbol{M}_0$ can be computed as:

$$\boldsymbol{F} = ([\boldsymbol{M}_0]_{:,1:n} - \bar{\boldsymbol{a}}\boldsymbol{1}_p^T)[\boldsymbol{B}]_{:,1:n}^{-1}, \tag{7}$$

where $[\boldsymbol{M}_0]_{:,1:n} = [\boldsymbol{m}_1, \ldots, \boldsymbol{m}_n] \in \mathbb{R}^{n \times n}$ and $[\boldsymbol{B}]_{:,1:n} = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_n] \in \mathbb{R}^{n \times n}$ are square matrices with full rank, representing the first n columns of matrices $\boldsymbol{M}_0$ and $\boldsymbol{B}$ respectively.

References

[1] C.-Y. Chi, W.-C. Li, and C.-H. Lin, *Convex Optimization for Signal Processing and Communications: From Fundamentals to Applications.* Boca Raton, FL, USA: CRC Press, 2017.

[2] W.-K. Ma, J. M. Bioucas-Dias, T.-H. Chan, N. Gillis, P. Gader, A. J. Plaza, A. Ambikapathi, and C.-Y. Chi, "A signal processing perspective on hyperspectral unmixing: Insights from remote sensing," *IEEE Signal Processing Magazine*, vol. 31, no. 1, pp. 67–81, 2014.

[3] S. Wold, K. Esbensen, and P. Geladi, "Principal component analysis," *Chemometrics and Intelligent Laboratory Systems*, vol. 2, no. 1, pp. 37–52, Aug. 1987.