Dual Simplex Volume Maximization for Simplex-Structured Matrix Factorization

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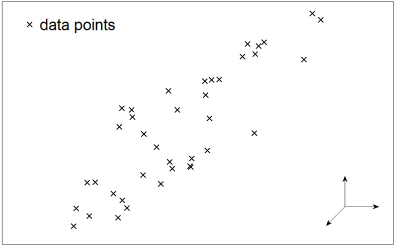
Low-Rank Nonnegative Matrix Factorization

Dimensionality reduction and Constrained Low-Rank Matrix Approximations

- Given n data points m_j $(j = 1, 2, \ldots, n)$, we would like to understand the underlying structure of this data through linear dimensionality reduction: find a set of r basis vectors u_k $(1 \leq k \leq r)$ so that for some weights v_{kj}
- This is **equivalent** to the low-rank approximation of matrix M:

$$M = [m_1\, m_2\, \ldots\, m_n] \;\approx\; [u_1\, u_2\, \ldots\, u_r]\,[v_1\, v_2\, \ldots\, v_n] \;=\; UV$$

m_j



- How to measure the **error** $||M - UV||$?

  Ex. PCA/truncated SVD use $||X||$ or $||X||_F^2$.

- What **constraints** should the factors $U \in \Omega_U$ and $V \in \Omega_V$ satisfy?

  Ex. PCA has no constraints, k-means a single '1' per column of V.

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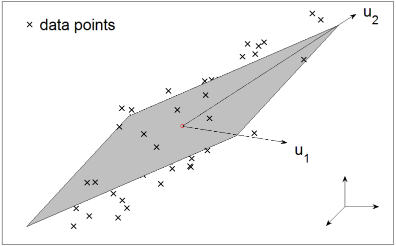

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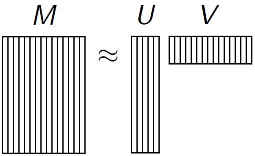

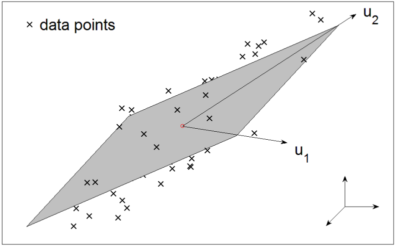

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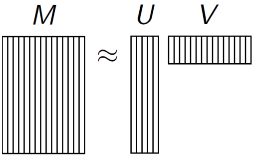

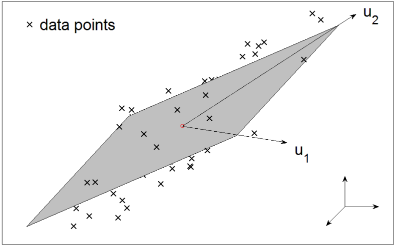

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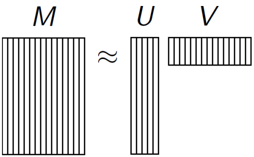

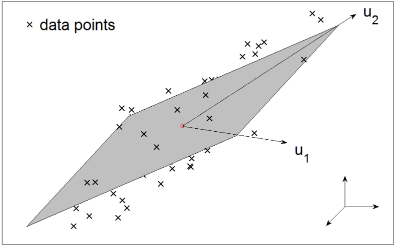

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Nonnegative Matrix Factorization (NMF)

Given a matrix $M \in \mathbb{R}_+^{p \times n}$ and a factorization rank $r \ll \min(p, n)$, find $U \in \mathbb{R}_+^{p \times r}$ and $V \in \mathbb{R}_+^{r \times n}$ such that

$$\min_{U \geq 0, V \geq 0} ||M - UV||_F^2 = \sum_{i,j} (M - UV)_{ij}^2 \qquad \text{(NMF)}$$

NMF is a linear dimensionality reduction technique for nonnegative data :

$$\underbrace{M(:,i)}_{\geq 0} \approx \sum_{k=1}^{r} \underbrace{U(:,k)}_{\geq 0} \underbrace{V(k,i)}_{\geq 0} \quad \text{for all } i$$

Why nonnegativity?

→ **Interpretability**: Nonnegativity constraints lead to easily interpretable factors (and a sparse and part-based representation)
→ **Many applications.** image processing, text mining, audio source separation, recommender systems, hyperspectral unmixing, community detection, clustering, etc.

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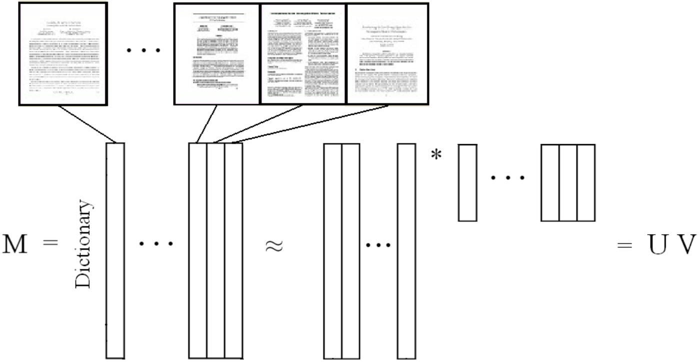
Application 1: topic recovery and document classification



- $M_{i,j}$ are the frequencies of word i in document j
- The columns $U_{:,k}$ represent the topics in the documents
- Weights in $V_{:,j}$ allow to assign each document j to its corresponding topics

Lee, D.D., Seung, H.S.: Learning the parts of objects by non-negative matrix factorization. Nature 401, 788–791 (1999)

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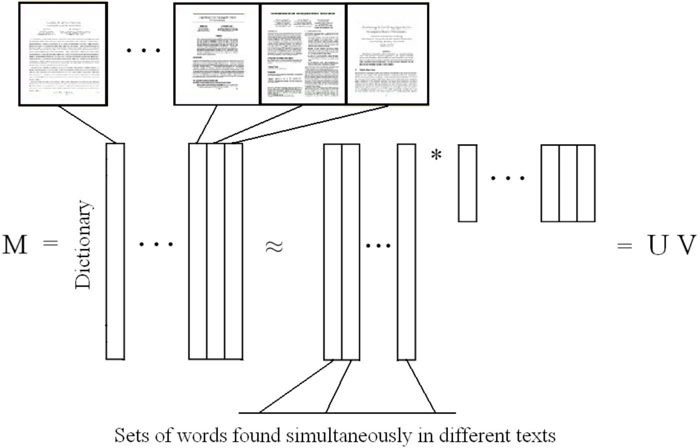

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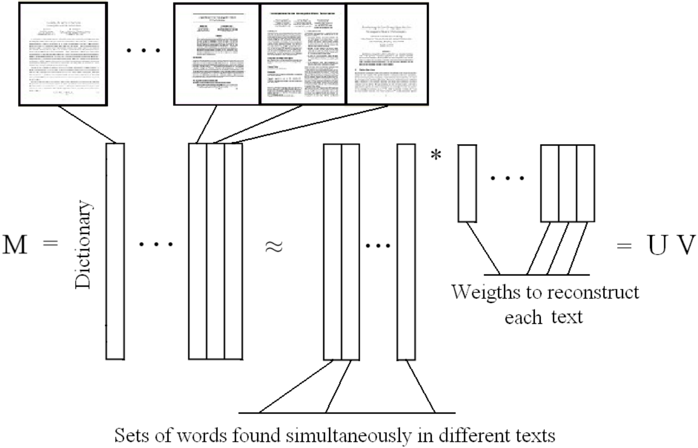

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Application 2: recommender systems

In some cases, some entries are missing/unknown

For example, we would like to predict how much someone is going to like a movie based on its movie preferences (e.g., 1 to 5 stars) :

$$\text{Movies} \quad \overset{\text{Users}}{\begin{bmatrix} 2 & 3 & 2 & ? & ? \\ ? & 1 & ? & 3 & 2 \\ 1 & ? & 4 & 1 & ? \\ 5 & 4 & ? & 3 & 2 \\ ? & 1 & 2 & ? & 4 \\ 1 & ? & 3 & 4 & 3 \end{bmatrix}}$$

Movies ratings are modeled as linear combinations of 'feature' movies (related to the genres - child oriented, serious vs. escapist, thriller, romantic, etc.)

$$\underbrace{M(i,:)}_{\text{movie } i} \approx \sum_{k=1}^{r} \underbrace{U(i,k)}_{\text{weights}} \underbrace{V(k,:)}_{\text{genre } k}$$

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For example, using a rank-2 factorization on the Netflix dataset, female vs. male and serious vs. escapist behaviors were extracted

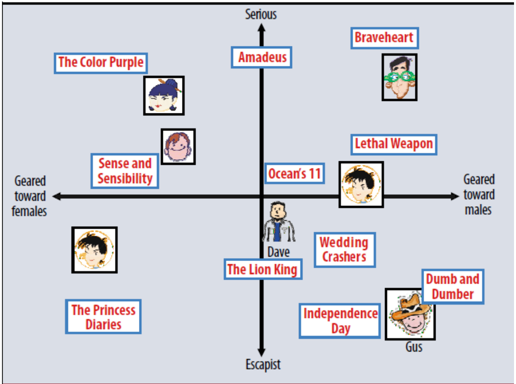

Figure 2. A simplified illustration of the latent factor approach, which characterizes both users and movies using two axes—male versus female and serious versus escapist.

Koren, Bell, Volinsky, *Matrix Factorization Techniques for Recommender Systems, 2009*
Winners of the Netflix prize 1,000,000$

Simplex-Structured Matrix Factorization

Geometric interpretation of exact NMF

Given $M = UV$, one can scale M and U such that they become column stochastic implying that V is column stochastic:

$$M = UV \iff M' = MD_M = (UD_U)(D_U^{-1}VD_M) = U'V'$$

The columns of M' are convex combinations of the columns of U':

$$M'_{:j} = \sum_{i=1}^{k} U'_{:i} V'_{ij} \quad \text{with} \quad \sum_{i=1}^{k} V'_{ij} = 1 \ \forall j, \ V'_{ij} \geq 0 \, \forall ij$$

In other terms

$$\text{conv}(M') \quad \subseteq \quad \text{conv}(U') \quad \subseteq \quad \Delta^n,$$

where $\text{conv}(X)$ is the convex hull of the columns of X, and $\Delta^n = \{x \in \mathbb{R}^n \,|x \geq 0, \sum_{i=1}^n x_i = 1 \}$ is the unit simplex

Exact NMF $\equiv$ Find r points whose convex hull is nested between two given polytopes (Nested Polytope Problem)

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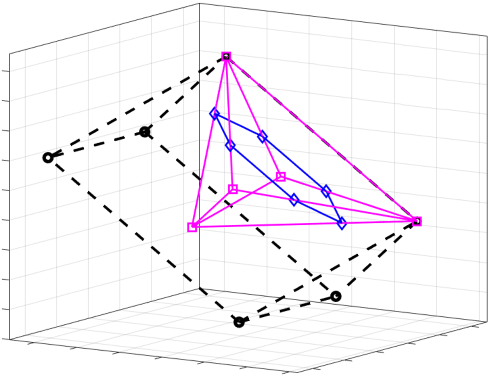

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from NMF to SSMF and back

Simplex-Structured Matrix Factorization requires V nonnegative and column stochastic: the columns of M are approximated as convex combinations of the basis vectors in U

$$\min_{U,V\geq 0} ||M - UV||_F^2 \quad : \quad V(:,j) \in \Delta := \{x \geq 0 : e^T x = 1\} \quad \forall j \qquad \text{(SSMF)}$$

Notice that we do not require M, U nonnegative or stochastic

Equivalently

$$\text{conv}(M) \quad \tilde{\subseteq} \quad \text{conv}(U)$$

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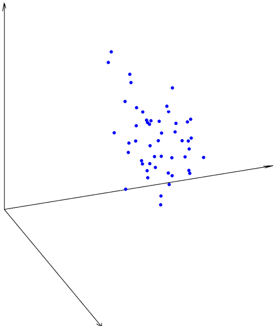

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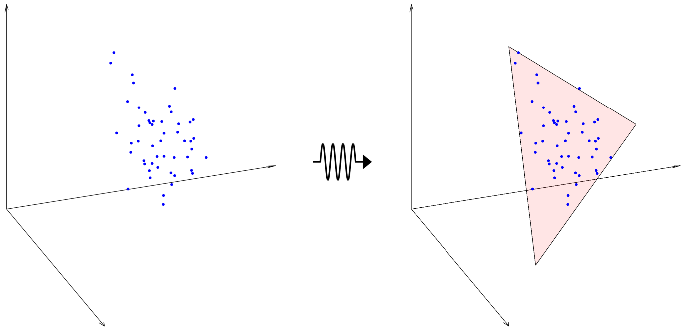
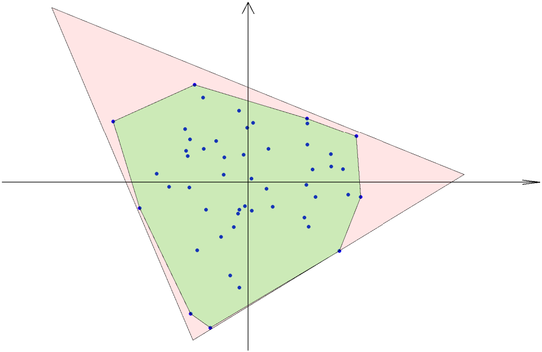


Solution to SSMF

$$Conv(M) \subseteq Conv(U) \qquad U \in \mathbb{R}^{m\times r}$$

Exists? **Yes** for $r \geq \text{dimaff}(M) + 1$ ...

but it is far from being ***Unique***



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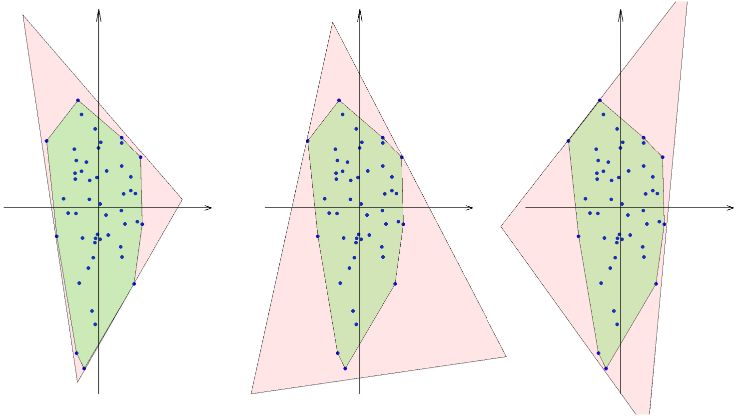

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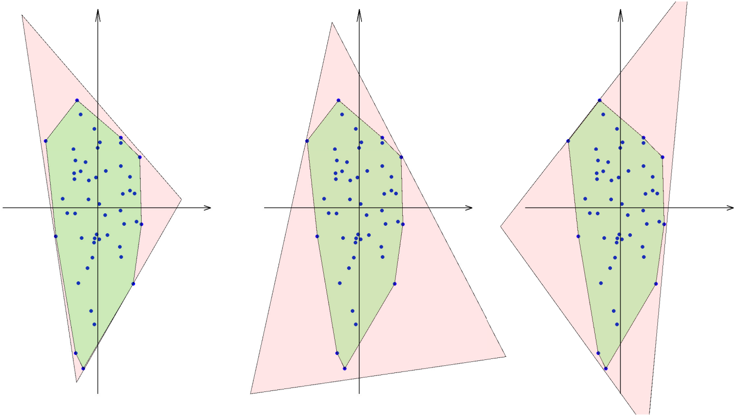

This is a problem for the **Interpretability** of the solution and the **Stability** of the algorithms

Application: Blind hyperspectral unmixing

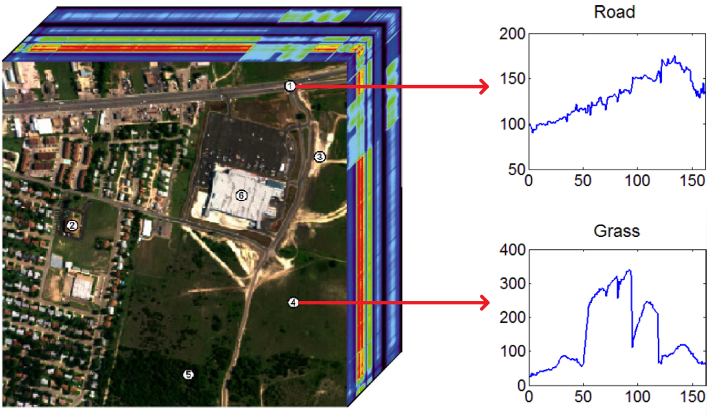

Figure 1: Urban hyperspectral image, 162 spectral bands and 307-by-307 pixels.

Problem. Identify the materials and classify the pixels

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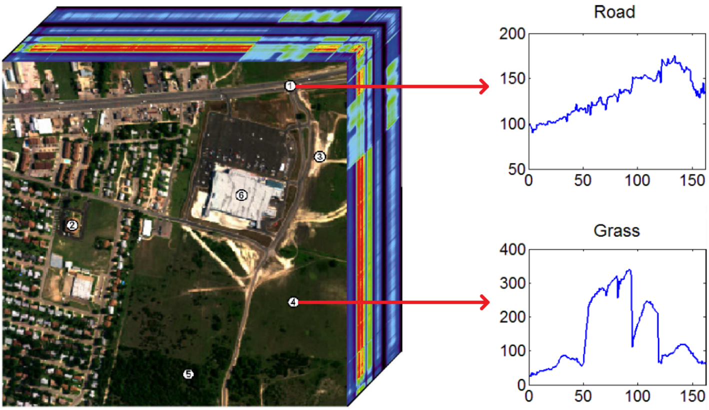

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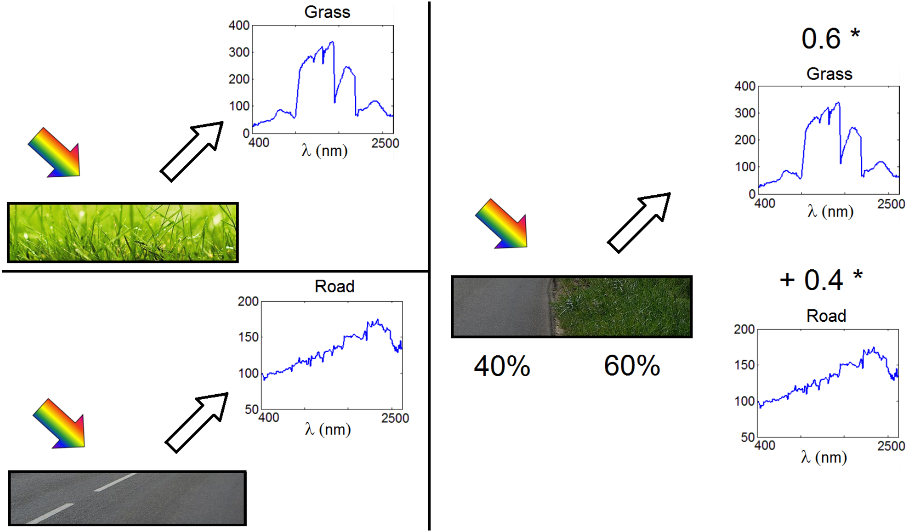

Urban hyperspectral image

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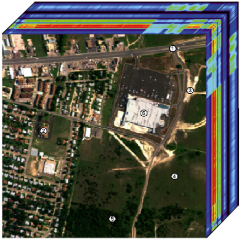

Figure 1: Decomposition of the Urban dataset

Zhu, F.: Hyperspectral unmixing: ground truth labeling, datasets, benchmark performances and survey. (2017) Arxiv

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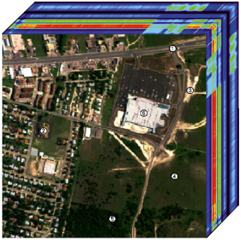

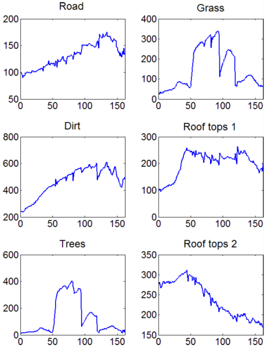

Figure 1: Decomposition of the Urban dataset

Zhu, F.: Hyperspectral unmixing: ground truth labeling, datasets, benchmark performances and survey. (2017) Arxiv

Urban hyperspectral image

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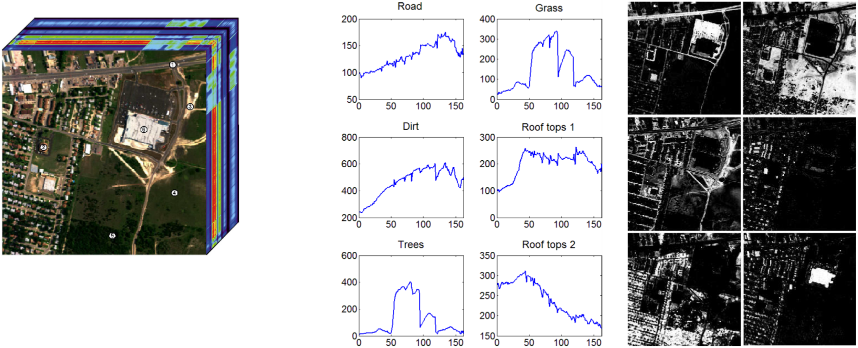

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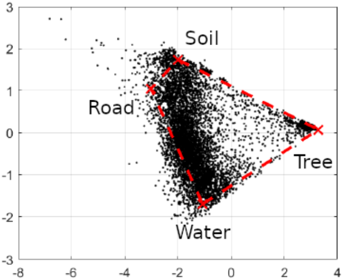
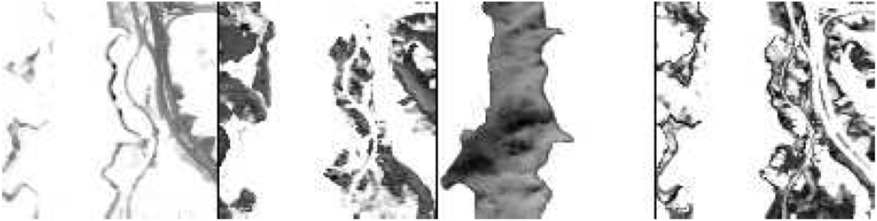
Urban hyperspectral image

Jasper Ridge Data set





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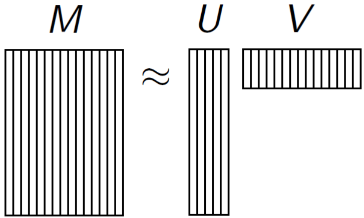
Separability and Successive Projections Algorithm

Separability Assumption

Separability of M: for an r-index set $\mathcal{K}$ and a V column stochastic, $M = \underbrace{M(:,\mathcal{K})}_{U} V$



Arora, Ge, Kannan, Moitra, *Computing a Nonnegative Matrix Factorization – Provably*, STOC 2012

If U is full rank, then the separability of $M = UV$ can be expressed as either

- U is a subset of the columns of M
- $V \in \mathbb{R}_+^{r \times n}$ has I_r as submatrix (up to permutation)
- $\text{conv}(U) = \text{conv}(M)$, so
  $M = \widetilde{U}\widetilde{V} \implies \text{conv}(U) \subseteq \text{conv}(\widetilde{U})$

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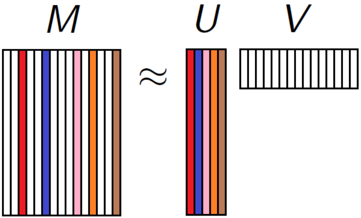

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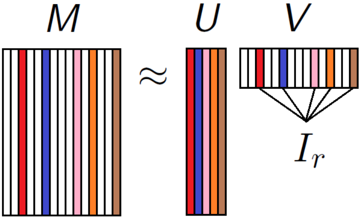

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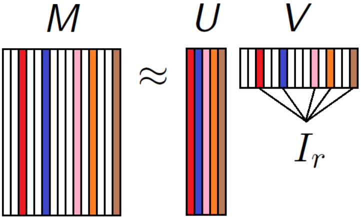

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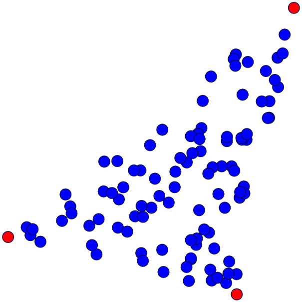

Successive Projection Algorithm (SPA)

Given $M = UV$ separable, U full column rank equal to r, repeat for r times:

1: Find $j^* = \text{argmax}_j ||M(:,j)||$ and add it to $\mathcal{K}$

2: $M \leftarrow \left(I - uu^T\right) M$ where $u = M(:,j^*)/||M(:,j^*)||$

The solution will be $U = M(:,\mathcal{K})$ and $V = U^\dagger M$

Araújo, U., Saldanha, B., Galvão, R., Yoneyama, T., Chame, H., Visani, V.: The successive projections algorithm for variable selection in spectroscopic multicomponent analysis. Chemometrics and Intelligent Laboratory Systems 57 (2001)

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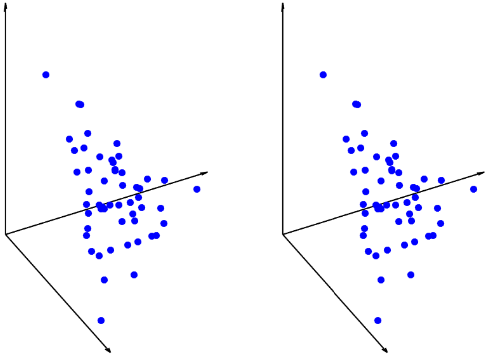

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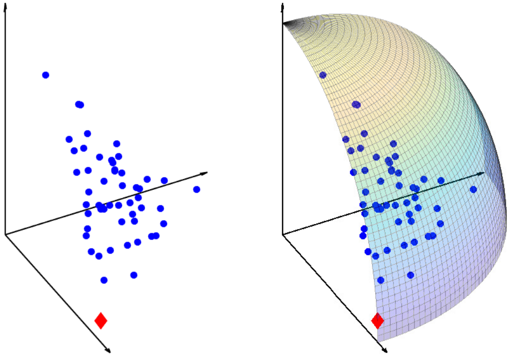

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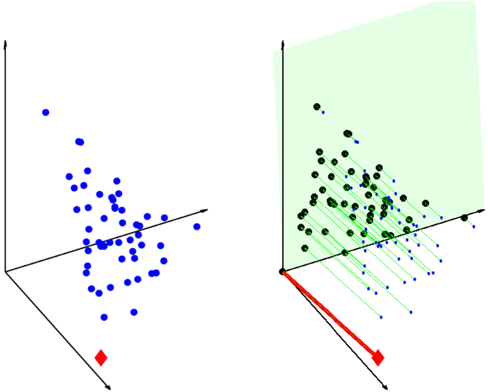

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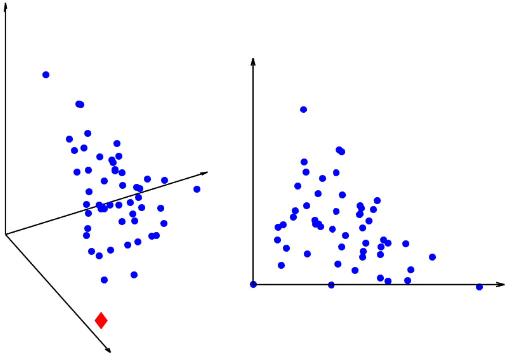

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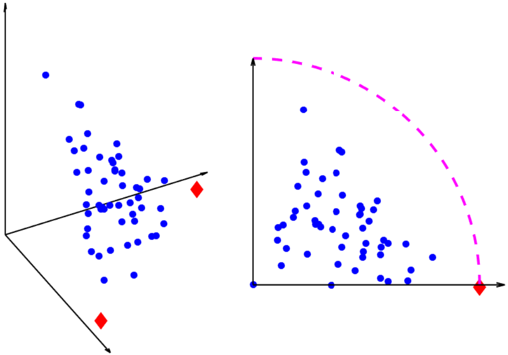

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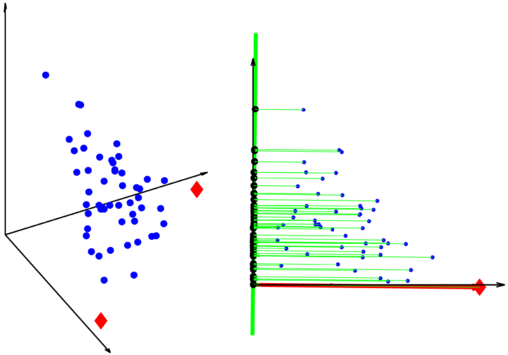

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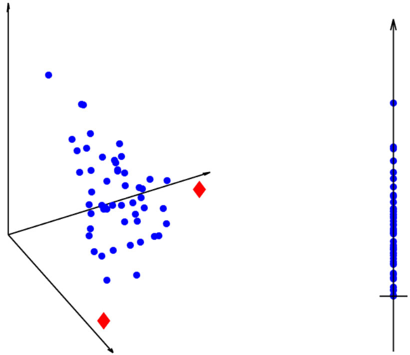

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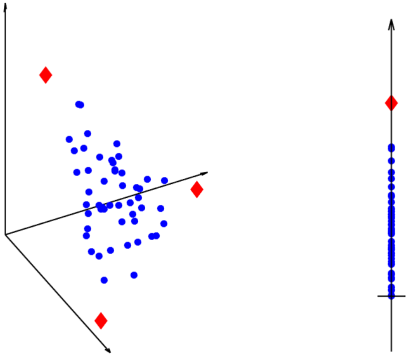

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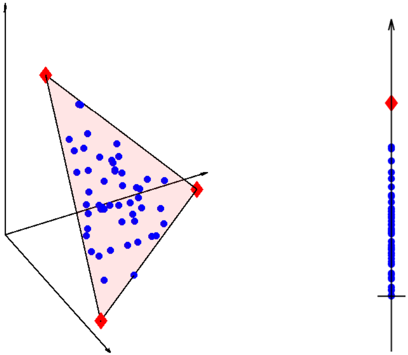

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Successive Projection Algorithm (SPA)

Perturbation robustness: suppose $M = UV + N$ with UV separable, U full rank and each column of N with norm at most ε

- If $\varepsilon \leq \mathcal{O}(\sigma_r(U)/\mathcal{K}(U)^2)$ then SPA extract a matrix $\widetilde{U}$ such that

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Gillis, N., Vavasis, S.A.: Fast and robust recursive algorithms for separable nonnegative matrix factorization. IEEE Transactions on Pattern Analysis and Machine Intelligence 36(4), 698–714 (2013)

Barbarino G, Gillis N.: On the Robustness of the Successive Projection Algorithm, (2024) Arxiv

Variants to improve robustness to perturbations and outliers:

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Gillis, N., Ma, W.K.: Enhancing pure-pixel identification performance via preconditioning. SIAM Journal on Imaging Sciences 8(2), 1161–1186 (2015)

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Gillis, N., Vavasis, S.A.: Semidefinite programming based preconditioning for more robust near-separable nonnegative matrix factorization. SIAM Journal on Optimization 25(1), 677–698 (2015)

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Vu Thanh, O., Nadisic, N., Gillis, N.: Randomized successive projection algorithm, GRETSI (2022).

Nadisic, N., Gillis, N., Kervazo, C.: Smoothed separable nonnegative matrix factorization. Linear Algebra and its Applications 676, 174–204 (2023).

Rank Deficient case: SNPA

What if $M = UV$ is separable but U is rank deficient?

SNPA: Successive Nonnegative Projection Algorithm

Modify the projection step as

1: Project the original M on $\text{conv}(M(:,\mathcal{K}))$ to obtain M_p

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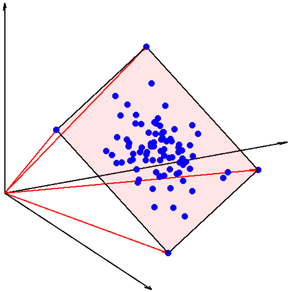
When $M_p = 0$, return $U = M(:,\mathcal{K})$



- ✓ Can handle the deficient rank case $\text{rk}(U) < r$
- × The bound on the error is $\mathcal{O}(\varepsilon \widetilde{\mathcal{K}}(U)^3)$
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Gillis, N.: Successive nonnegative projection algorithm for robust nonnegative blind source separation. SIAM Journal on Imaging Sciences 7(2), 1420–1450 (2014)

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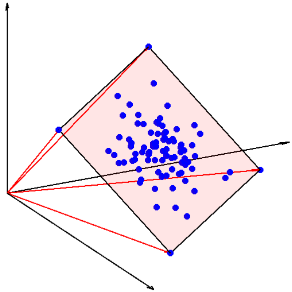

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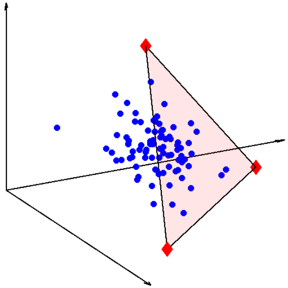

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Gillis, N.: Successive nonnegative projection algorithm for robust nonnegative blind source separation. SIAM Journal on Imaging Sciences 7(2), 1420–1450 (2014)

Rank Deficient case: SNPA

What if $M = UV$ is separable but U is rank deficient?

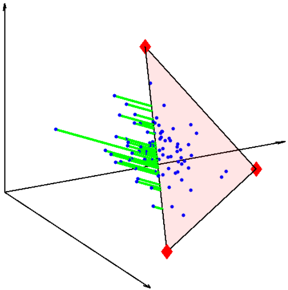
SNPA: Successive Nonnegative Projection Algorithm

Modify the projection step as

1: Project the original M on $\text{conv}(M(:,\mathcal{K}))$ to obtain M_p

2: Find $j^* = \text{argmax}_j ||M(:,j) - M_p(:,j)||$ and add it to $\mathcal{K}$

When $M_p = 0$, return $U = M(:,\mathcal{K})$



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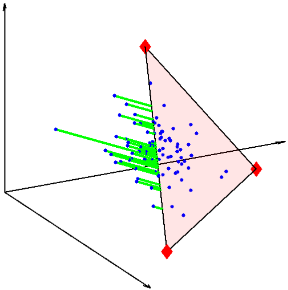

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SSC and Minimum Volume

Sufficiently Scattered Condition

Separability leads to fast and robust algorithms, but it is a strong assumption

A column stochastic matrix V is sufficiently scattered if

SSC1: $\mathcal{C} := \{x \mid 1 = e^\top x \geq \sqrt{r-1}\|x\|\} \subseteq \text{conv}(V)$

SSC2: if Q is orthogonal and $\text{conv}(V) \subseteq \text{conv}(Q)$ then Q is a permutation matrix

Tl;dr: $\mathcal{C} \subseteq \text{conv}(V)$

Notice: Separability $\implies$ V contains I as submatrix $\implies$ $\mathcal{C} \subseteq \Delta = \text{conv}(V)$ $\implies$ SSC

Theorem

If $M = UV$ with V SSC, U full rank exists, then it is the **unique solution** to

$$\min_{U \in \mathbb{R}^{m \times r}} Vol(U) : Conv(M) \subseteq Conv(U)$$

Notice2: SSC1 ensures the minimality, SSC2 ensures the uniqueness

Fu, X., Ma, W.K., Huang, K., Sidiropoulos, N.D.: Blind separation of quasi-stationary sources: exploiting convex geometry in covariance domain. IEEE Transactions on Signal Processing 63(9), 2306–2320 (2015)

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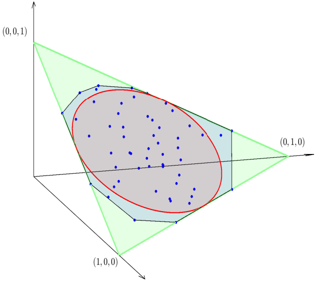

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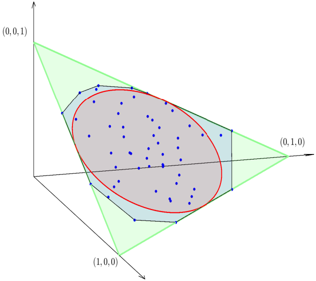

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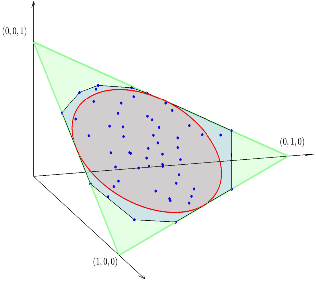

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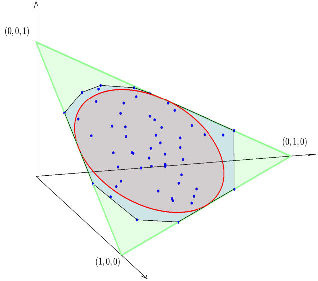

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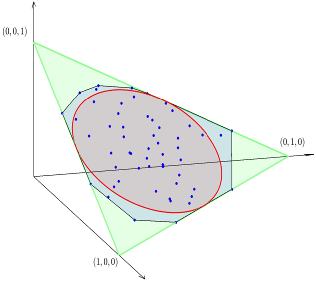

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Simplex Volume Minimization

Exact Case:

$$\min_{U \in \mathbb{R}^{m \times r}} Vol(U) \;:\; Conv(M) \subseteq Conv(U)$$

Inexact Case:

$$\min_{U,V} \|M - UV\|_F^2 + \lambda \log\det(U^\top U) \;:\; V \text{ column stochastic}$$

Alternating Method: Given $(\widetilde{U}, \widetilde{V})$ initial approximation,

Update of U

$$\log\det(A) \leq \langle B^{-1}, A \rangle + \log\det(B) - r$$

with $=$ iff $B = A \succ 0$

$$\|M - U\widetilde{V}\|_F^2 + \lambda \log\det(U^\top U) \leq \langle UU^\top, E \rangle - \langle U, C \rangle + b$$

where $E = \lambda(\widetilde{U}^\top \widetilde{U})^{-1} + \widetilde{V}\widetilde{V}^\top$, $C = 2M\widetilde{V}^T$ and b do not depend on U

$$\min_U \sum_i u_i^\top E u_i - c_i^\top u_i$$

are m quadratic and strongly convex optimization problems on the rows of U

Update of V

$$\|M - \widetilde{U}V\|_F^2 + \lambda \log\det(\widetilde{U}^\top \widetilde{U}) = \langle VV^\top, E \rangle - \langle V, C \rangle + b$$

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Leplat, V., Ang, A.M., Gillis, N.: Minimum-volume rank-deficient nonnegative matrix factoriza- tions. In: IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), pp. 3402–3406 (2019)

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Facet Identification

PCA Preprocessing: Given $\widetilde{M} = \widetilde{U}V \in \mathbb{R}^{m\times n}$ and U of rank r we can always reduce to

$$Q(\widetilde{M} - ze^\top) = Q(\widetilde{U} - ze^\top)V \in \mathbb{R}^{(r-1)\times n}$$

In other words, we have to find a simplex: r vertices in $r-1$ dimensions

$$Conv(U) = \cap_{i=1}^{r}\mathcal{S}_i \quad \text{where} \quad \mathcal{S}_i := \{x : \theta_i^T x \leq 1\}$$

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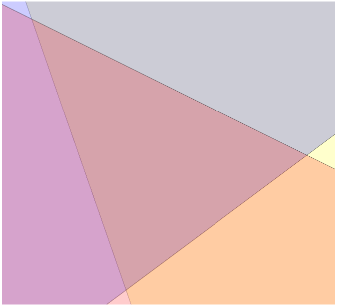
MVIE *Maximum Volume Inscribed Ellipsoid*

Enumerates the facets of $Conv(M)$, very expensive

GFPI *Greedy Facet-based Polytope Identification*

Mixed integer programming, also expensive



In order to deal with facets GFPI works in the **Polar Space**

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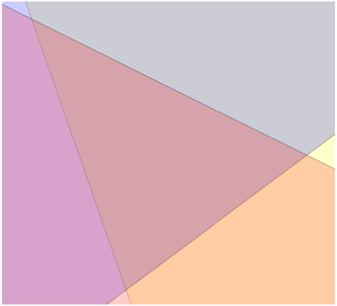

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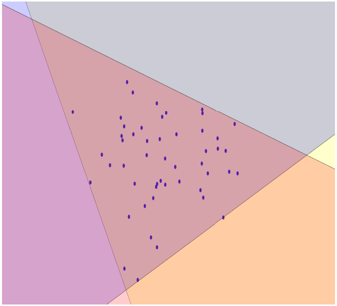

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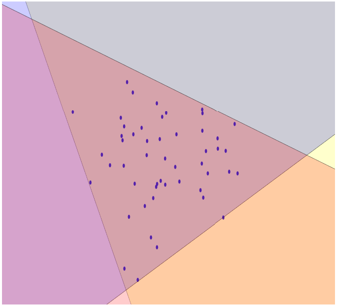
Lin, C.H., Wu, R., Ma, W.K., Chi, C.Y., Wang, Y.: Maximum volume inscribed ellipsoid: A new simplex- structured matrix factorization framework via facet enumeration and convex optimization. SIAM Journal on Imaging Sciences 11 (2018)



GFPI *Greedy Facet-based Polytope Identification*

Mixed integer programming, also expensive

In order to deal with facets GFPI works in the **Polar Space**

Facet Based Algorithms

PCA Preprocessing: Given $\widetilde{M} = \widetilde{U}V \in \mathbb{R}^{m \times n}$ and U of rank r we can always reduce to

$$Q(\widetilde{M} - ze^\top) = Q(\widetilde{U} - ze^\top)V \in \mathbb{R}^{(r-1)\times n}$$

In other words, we have to find a simplex: r vertices in $r-1$ dimensions

$$Conv(U) = \cap_{i=1}^{r} \mathcal{S}_i \quad \text{where} \quad \mathcal{S}_i := \{x : \theta_i^T x \leq 1\}$$

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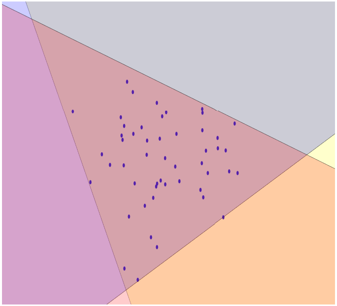
Abdolali, M., Gillis, N.: Simplex-structured matrix factorization: Sparsity-based identifiability and provably correct algorithms. SIAM Journal on Mathematics of Data Science 3(2), 593–623 (2021)



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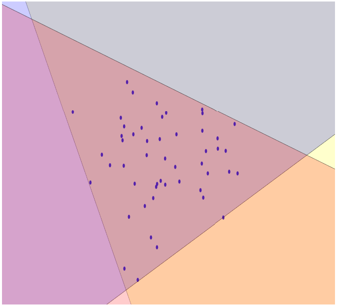

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Polarity

$$\mathcal{S} \subseteq \mathbb{R}^{r-1} \qquad \mathcal{S}^* := \{\theta : \theta^T x \leq 1 \; \forall x \in \mathcal{S}\}$$

- Swaps points and hyperplanes

$$\{x : \theta^T x = 1\} \rightsquigarrow \theta$$

- Sends simplexes into simplexes
- It is an involution for convex sets
- **Reverses Containments**

$$Conv(M) \subseteq Conv(U) \iff Conv(U)^* \subseteq Conv(M)^*$$

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We can thus seek the simplex Θ with **maximum volume** inside $Conv(M)^*$ as in

$$\max_{\theta \in \mathbb{R}^{r-1 \times r}} Vol(\Theta) \quad : \quad \Theta^T M \leq 1 \qquad (MaxVol)$$

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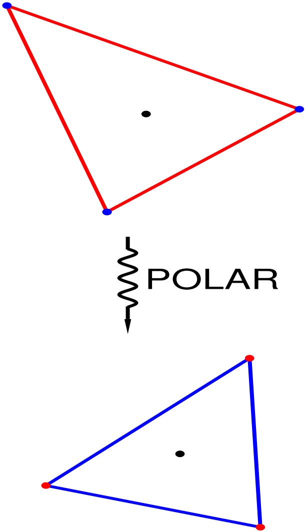

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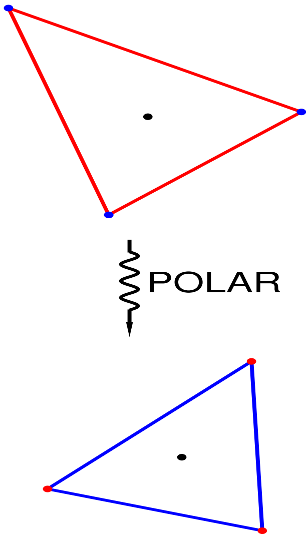

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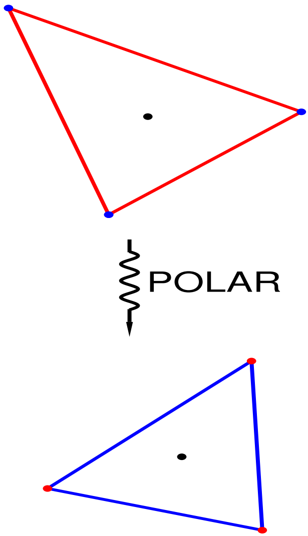

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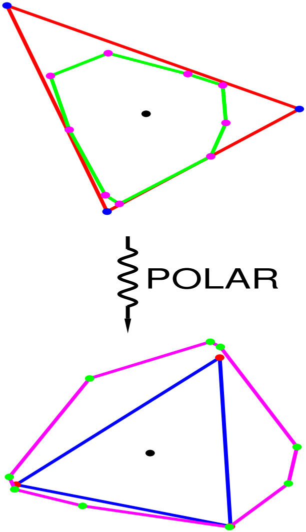

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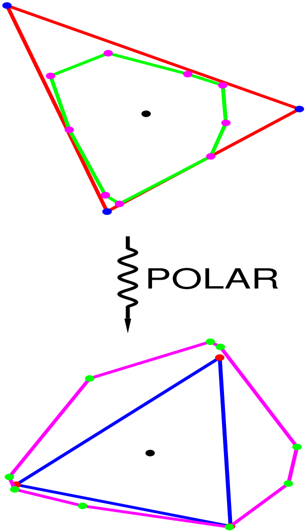

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Identifiability and η-Expansion

Theorem (M.A., G.B., N.G., 2023)

Let $M = UV \in \mathbb{R}^{r-\mathbf{1} \times n}$ SSC and for any $u \in \mathbb{R}^{r-\mathbf{1}}$ define

$$\mathcal{V}(u) := \max_{\Theta \in \mathbb{R}^{r-\mathbf{1} \times r}} Vol(\Theta) \quad : \quad \Theta^T(M - ue^T) \leq 1$$

Then $\mathcal{V}(u)$ is convex in u with unique minimum for $u = Ue/r$ and Θ polar of U

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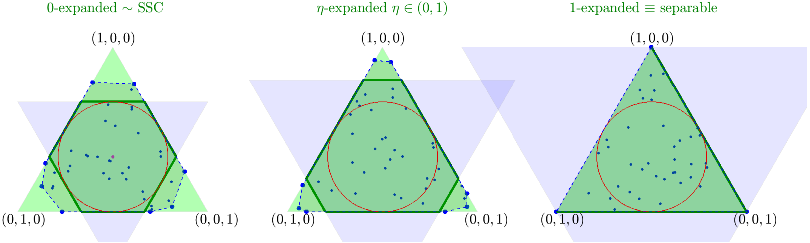

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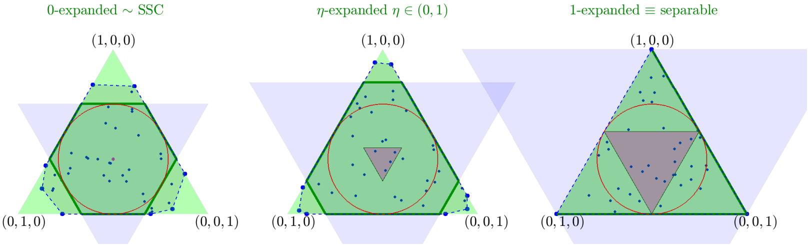

Theorem (M.A., G.B., N.G., 2023)

Let $M = UV \in \mathbb{R}^{r-1 \times n}$ be η-expanded and suppose $u = Uv$, $v \in \blacktriangledown$. Then

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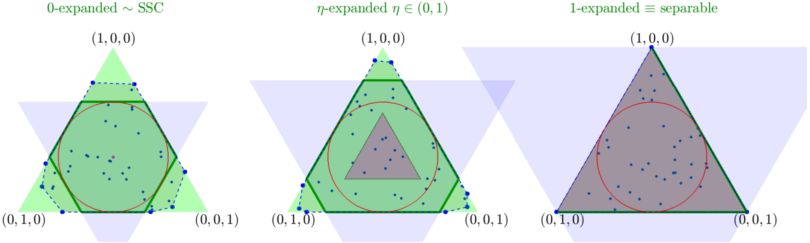

Conjecture (M.A., G.B., N.G., 2023)

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Maximum Volume in Dual

Algorithm Maximum Volume in the Dual (MV-Dual)

Input: Data matrix $\widetilde{M} \in \mathbb{R}^{m \times n}$ and a factorization rank r

Output: A matrix $\widetilde{U} \in \mathbb{R}^{m \times r}$ and a vector z such that $\widetilde{M} \approx z + \widetilde{U}V$ where V is column stochastic

1: Use PCA to reduce $\widetilde{M} = z + QM$ with $M \in \mathbb{R}^{r-\mathbf{1} \times n}$

2: Initialize $u_1 = Me/n$, $p = 1$ and $\Theta \in \mathcal{N}(0,1)^{r-\mathbf{1} \times r}$

3: **while** not converged: $p = 1$ or $\frac{\|u_p - u_{p-\mathbf{1}}\|_\mathbf{2}}{\|u_{p-\mathbf{1}}\|_\mathbf{2}} > 0.01$ **do**

4: Solve

$$\arg \max_{\Theta \in \mathbb{R}^{r-\mathbf{1} \times r}} Vol(\Theta) : \Theta^T (X - v_p e^T) \leq 1$$

via alternating optimization on the columns of Θ

5: Recover U by computing the polar of $Conv\,(\Theta)$

6: Let $u_{p+1} \leftarrow Ue/r$, and $p = p + 1$

7: **end while**

8: Compute $\widetilde{U} = QU$

Cost : PCA $\mathcal{O}(mnr)$ plus Maximization problem solver for a single column $\mathcal{O}(nr^2)$ times the number of iterations

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Use PCA to reduce $\widetilde{M} = z + QM$ with $M \in \mathbb{R}^{r-1 \times n}$

Initialize $u_1 = Me/n$, $p = 1$ and $\Theta \in \mathcal{N}(0,1)^{r-1 \times r}$

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    Solve

$$\arg \max_{\Theta \in \mathbb{R}^{r-1 \times r}, \Delta \in \mathbb{R}^{r \times n}} Vol(\Theta)^2 - \lambda \|\Delta\|_F^2 : \Theta^T (X - v_p e^T) \leq 1 + \Delta^T$$

    via alternating optimization on the columns of Θ, Δ

    Recover U by computing the polar of $Conv(\Theta)$

    Let $u_{p+1} \leftarrow Ue/r$, and $p = p + 1$

end while

Compute $\widetilde{U} = QU$

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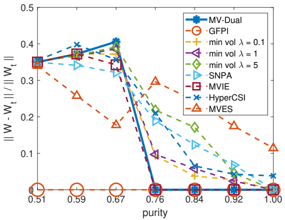
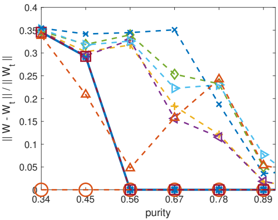
Experiments

Exact Case

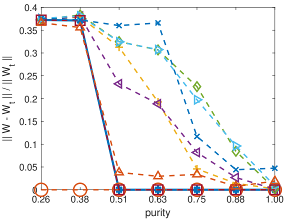
U^*, V^* ground truth $\quad ERR = \frac{\|U^* - U\|_F}{\|U^*\|_F} \quad$ purity $p = \max_{i,j} |V^*_{i,j}| = \eta + (1-\eta)\frac{2}{r}$



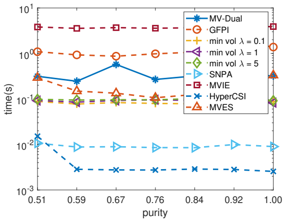
ERR for $r = 3,\ n = 30r$



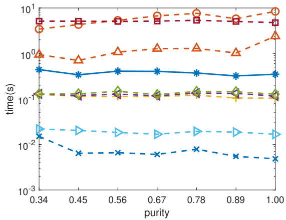
ERR for $r = 4,\ n = 30r$



ERR for $r = 5,\ n = 30r$



Time for $r = 3,\ n = 30r$



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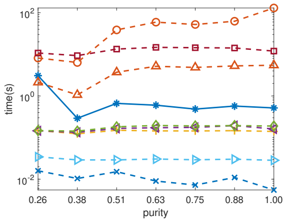

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Noisy Case

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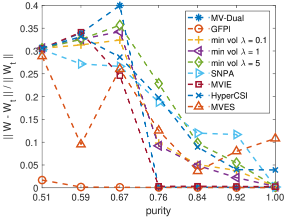
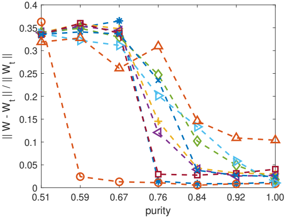


ERR for $r = 3$, SNR $= 60$



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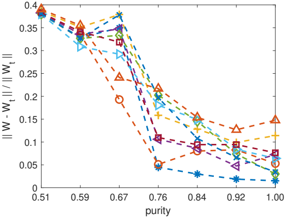

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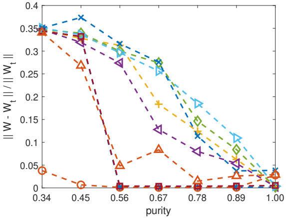

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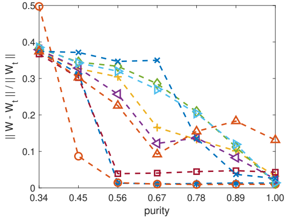

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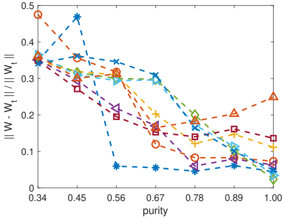

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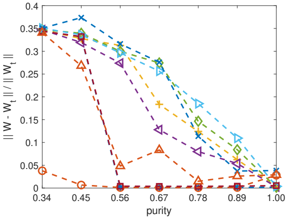

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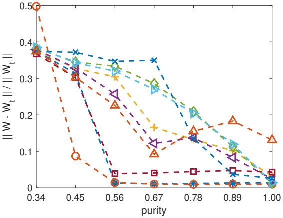

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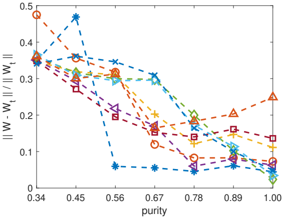
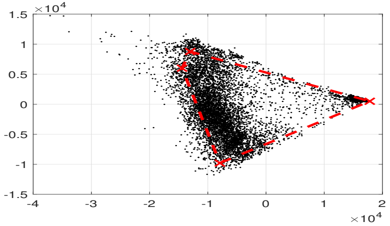


ERR for $r = 4$, SNR $= 30$

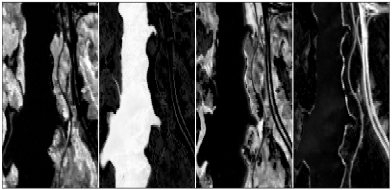
SNR	MVDual	GFPI	min vol $\lambda = 0.1$	min vol $\lambda = 1$	min vol $\lambda = 5$	SNPA	MVIE	HyperCSI	MVES
30	0.56±0.11	7.76±3.51	0.12±0.01	0.13±0.01	0.14±0.02	0.01±0.001	5.28±0.23	0.01±0.004	0.30±0.04
40	0.45±0.06	4.18±1.12	0.10±0.01	0.11±0.01	0.13±0.01	0.01±0.00	4.96±0.12	0.005±0.004	0.30±0.05
60	0.42±0.06	1.47±0.45	0.07±0.01	0.08±0.01	0.09±0.01	0.01±0.00	3.78±0.12	0.001±0.00	0.26±0.07

Unmixing Hyperspectral Imaging

$$\mathrm{MRSA}(x, y) = \frac{100}{\pi} \cos^{-1}\left(\frac{(x-\bar{x}e)^\top (y-\bar{y}e)}{\|x-\bar{x}e\|_2 \|y-\bar{y}e\|_2}\right) \qquad ERR = \sum_k \mathrm{MRSA}(U_k^*, U_k)$$



Projection of data points
and the symplex computed by MV-Dual



Abundance maps estimated by MV-Dual
From left to right: road, tree, soil, water

	SNPA	Min-Vol	HyperCSI	GFPI	MV-Dual
MRSA	22.27	6.03	17.04	4.82	3.74
Time (s)	0.60	1.45	0.88	100*	43.51

Comparing the performances of MV-Dual with the state-of-the-art SSMF algorithms on Jasper-Ridge data set. Numbers marked with * indicate that the corresponding algorithms did not converge within 100 seconds.

Thank You!

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