# Sparse Separable Nonnegative Matrix Factorization

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# Nonnegative Matrix Factorization (NMF)

NMF is a linear dimensionality reduction technique for nonnegative data.

Given a data matrix $M \in \mathbb{R}_+^{m \times n}$ and a rank $r \ll \min(m, n)$, find $W \in \mathbb{R}_+^{m \times r}$ and $H \in \mathbb{R}_+^{r \times n}$ such that $M \approx WH$.

In optimization terms, standard NMF is equivalent to:

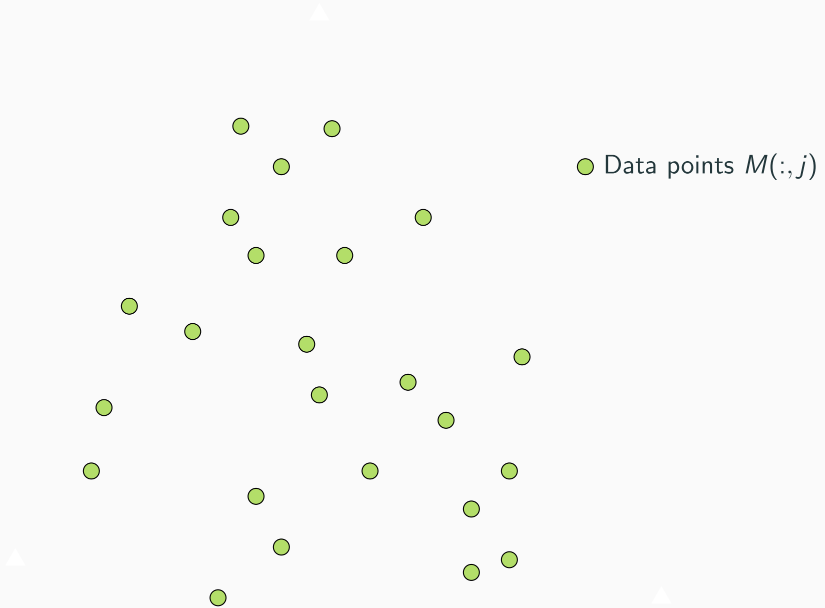
$$\min_{W \geq 0, H \geq 0} \|M - WH\|_F^2$$

# Nonnegative Matrix Factorization (NMF)

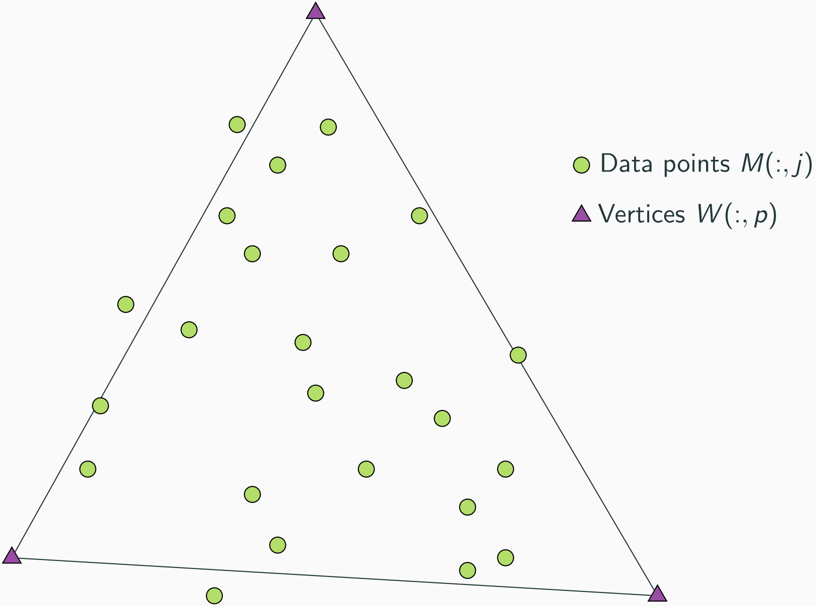
Why nonnegativity?

- More interpretable factors (part-based representation)
- Naturally favors sparsity
- Makes sense in many applications (image processing, hyperspectral unmixing, text mining, ...)

# NMF Geometry ($M \approx WH$)



# NMF Geometry ($M \approx WH$)



# Application – hyperspectral unmixing

$$\underbrace{M(:,j)}_{\text{spectral signature of j-th pixel}} \approx \sum_p \underbrace{W(:,p)}_{\text{spectral signature of p-th material}} \underbrace{H(p,j)}_{\text{abundance of p-th material in j-th pixel}}$$

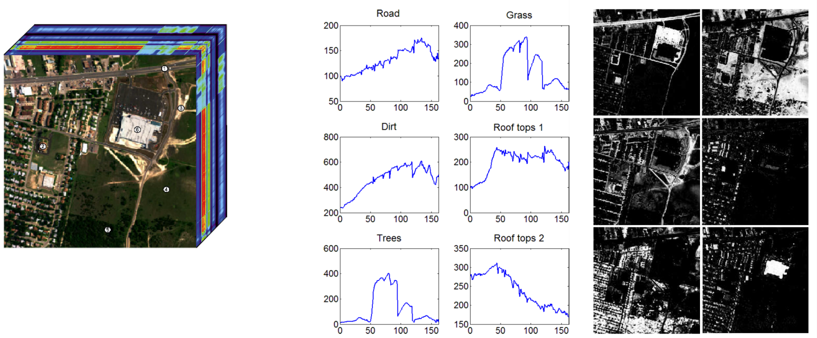
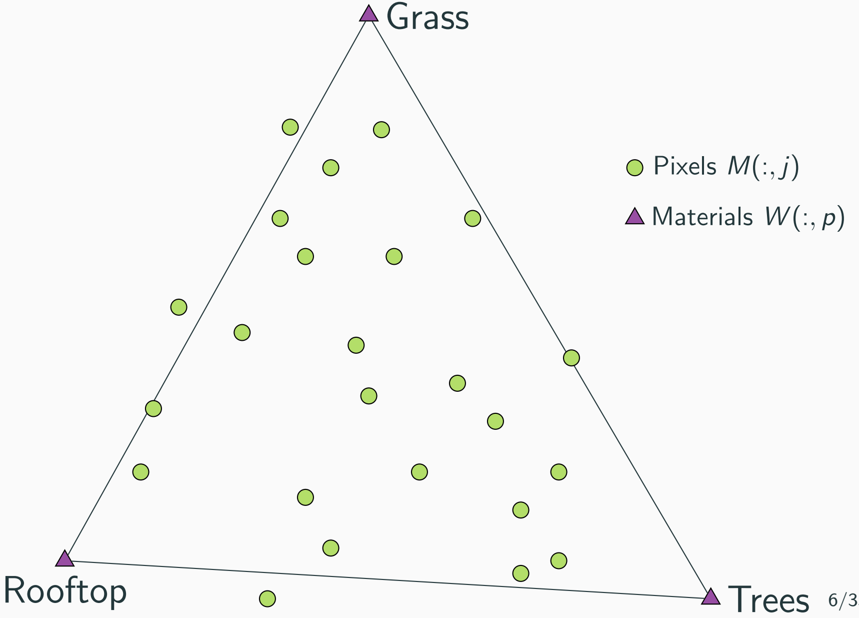



Image from Nicolas Gillis.

# Application – hyperspectral unmixing



# Starting point 1/2 – Separable NMF

- NMF is NP-hard [Vavasis, 2010].
- Under the separability assumption, it's solvable in polynomial time [Arora et al., 2012].

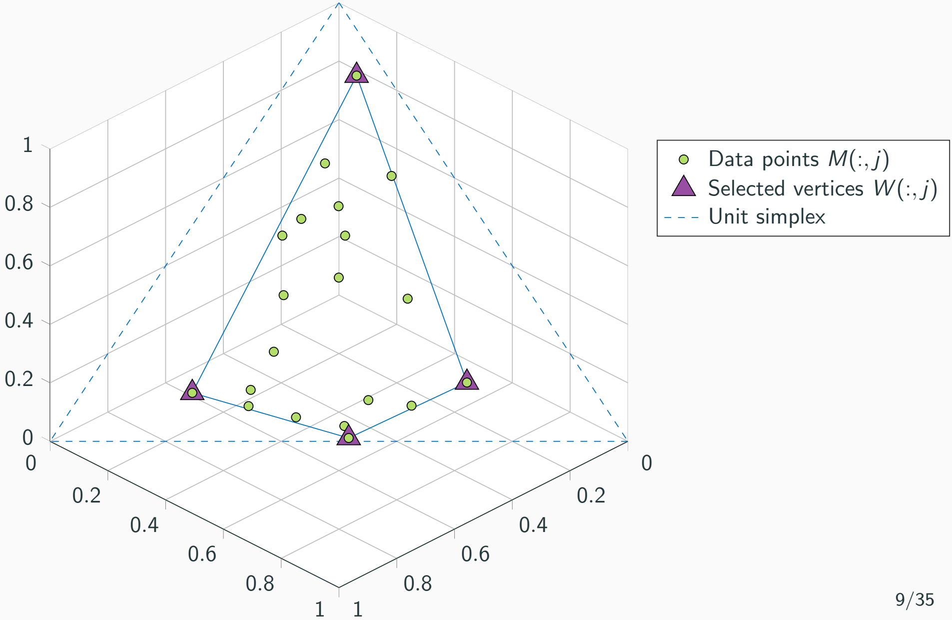
# Starting point 1/2 – Separable NMF

Separability:

- The vertices are selected among the data points
- In hyperspectral unmixing, equivalent to Pure-pixel assumption

| | |
|---|---|
| Standard NMF model | $M = WH$ |
| Separable NMF | $M = M(:, \mathcal{J})H$ |

# Separable NMF – Geometry

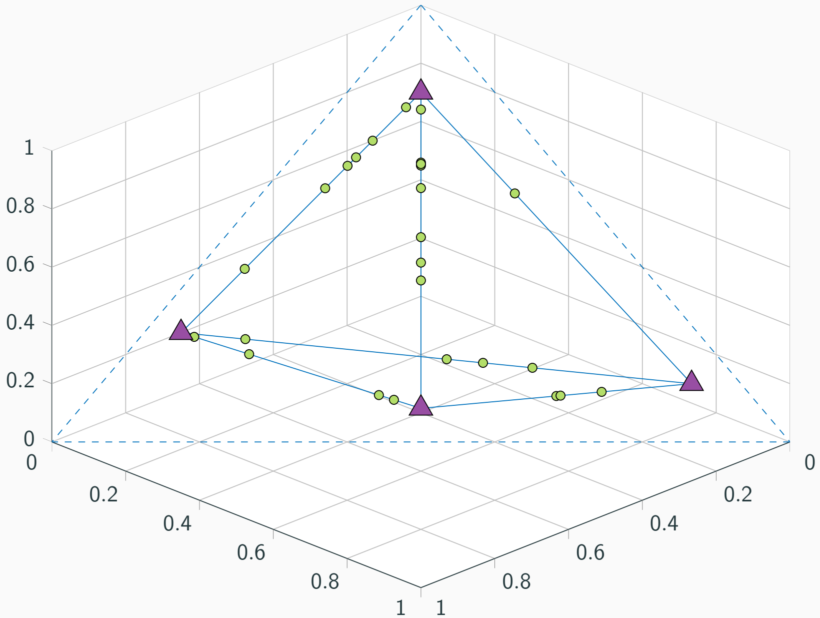


# Starting point 2/2 — k-Sparse NMF

$M = WH$ s.t. $H$ is column-wise $k$-sparse (for all $i$, $\|H(:,i)\|_0 \leq k$)

- Motivation $\rightarrow$ better interpretability
- Motivation $\rightarrow$ improve results using prior sparsity knowledge
- Ex: a pixel expressed as a combination of at most $k$ materials

# k-Sparse NMF – Geometry with $r = 4$ and $k = 2$



# Sum-up of our work

**What?** Combine two models, Separable NMF and k-Sparse NMF

**Why?** Underdetermined blind source separation

**How?** New algo based on SNPA and an exact k-Sparse NNLS solver (provably correct, and works in “real-life”)

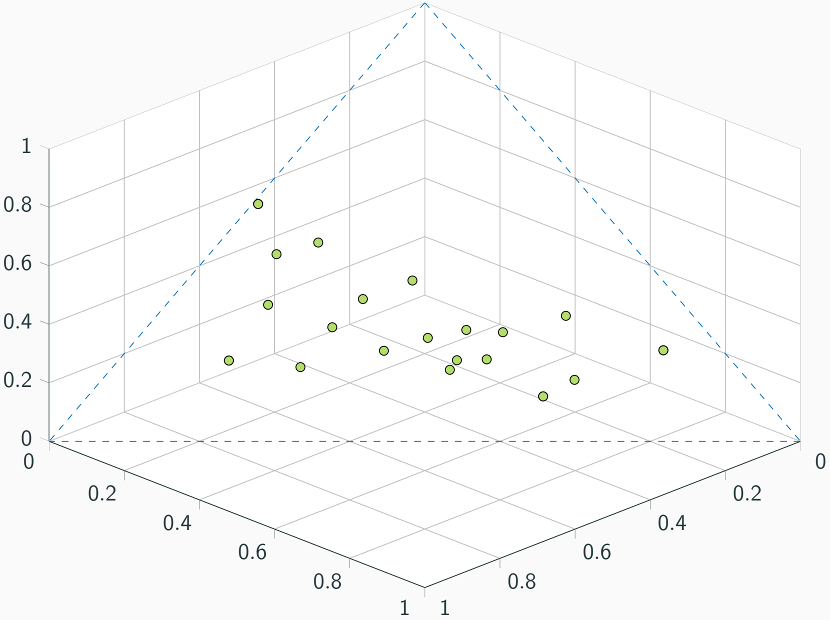
(End of introduction)

# Algorithm for Separable NMF – SNPA

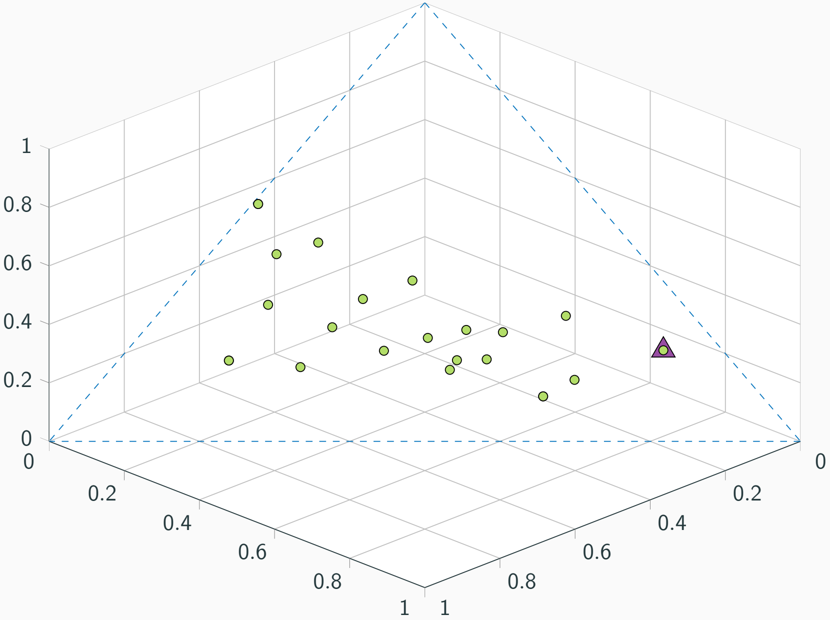
SNPA = Successive Nonnegative Projection Algorithm [Gillis, 2014]

- Start with empty $W$, and residual $R = M$
- Alternate between
  - Greedy selection of one column of $R$ to be added to $W$
  - Projection of $R$ on the convex hull of the origin and columns of $W$
- Stop when reconstruction error $= 0$ (or $< \epsilon$)

# SNPA



# SNPA



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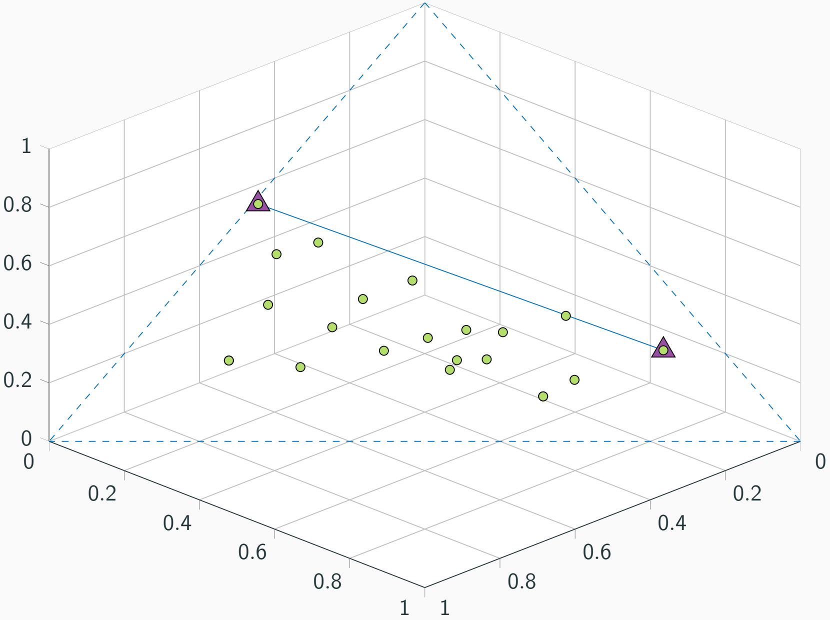

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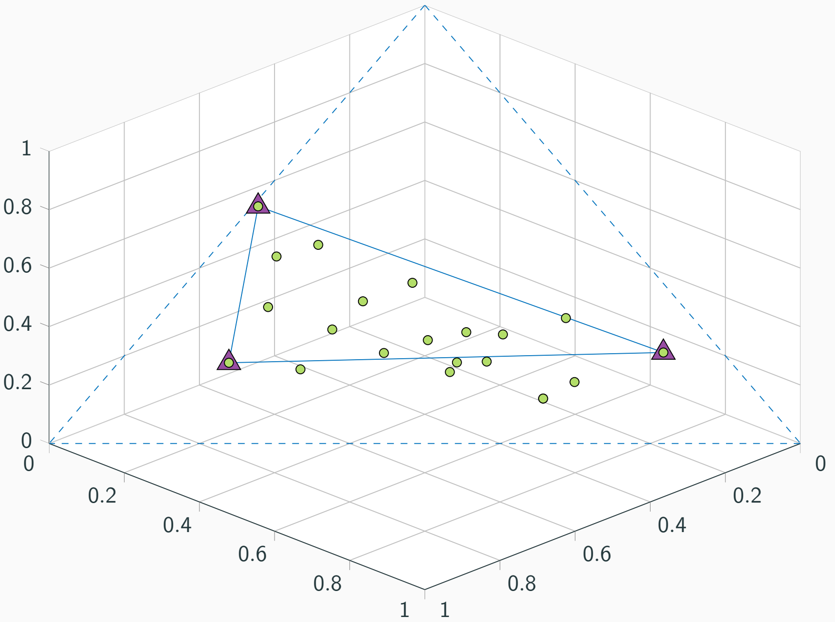
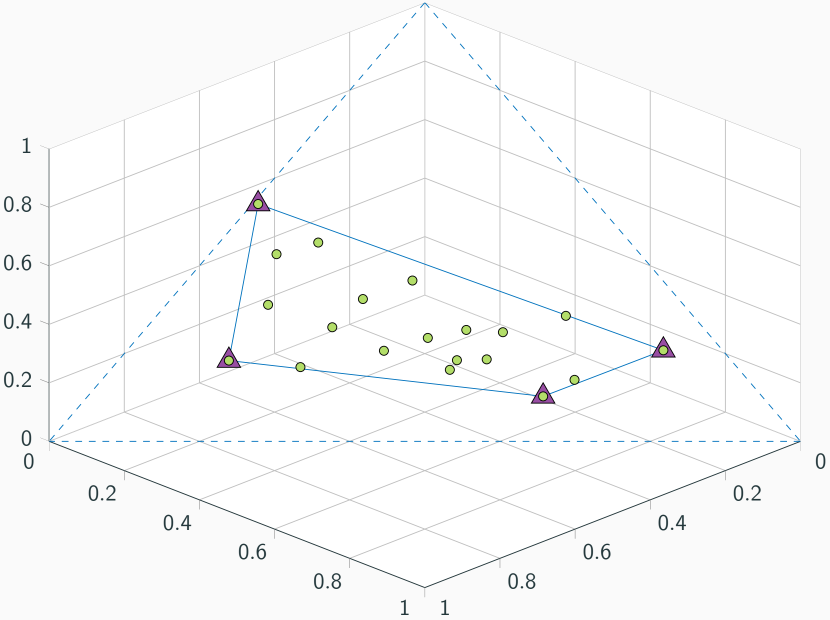


# SNPA

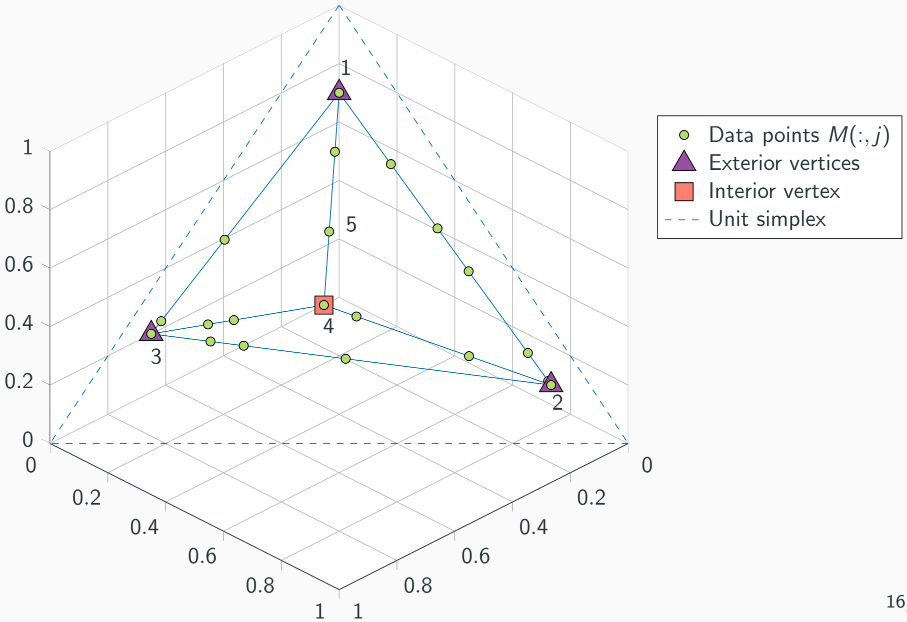


# Limitations of Separable NMF

What if one column of $W$ is a combination of others columns of $W$?

$\rightarrow$ Interior vertex

# Limitations of Separable NMF



## Limitations of Separable NMF

SNPA is unable to handle this case, the interior vertex is not identifiable.

However, if columns of $H$ are sparse (a data point is a combination of only $k < r$ vertices), this interior vertex may be identifiable.

# Sparse Separable NMF

Standard NMF model $M = WH$

Separable NMF $M = M(:, \mathcal{J})H$

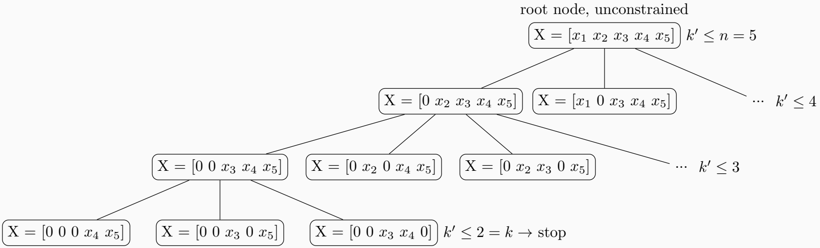
SSNMF $M = M(:, \mathcal{J})H$ s.t. for all $i$, $\|H(:, i)\|_0 \leq k$

# k-Sparse NMF

k-Sparse NMF is combinatorial ($\Leftrightarrow$ find the pattern of nonzero entries).

$\binom{r}{k}$ possible combinations.

Previous work: a branch-and-bound algorithm for Exact k-Sparse NNLS [Nadisic et al., 2020].



# Our approach for SSNMF

Replace the projection step of SNPA, from projection on convex hull to projection on $k$-sparse hull, done with our BnB solver $\Rightarrow$ kSSNPA.

kSSNPA

- Identifies all interior vertices
- May also identify wrong vertices (explanation to come!)

$\Rightarrow$ kSSNPA can be seen as a screening technique to reduce the number of points to check.

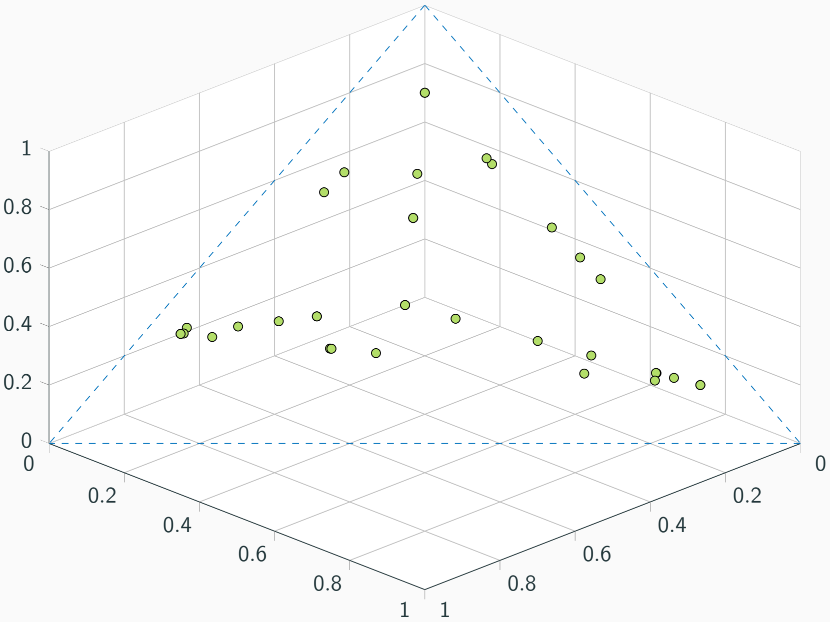
# Our approach for SSNMF

In a nutshell, 3 steps:

1. Identify exterior vertices with SNPA
2. Identify candidate interior vertices with kSSNPA
3. Discard bad candidates, those that are $k$-sparse combinations of other selected points (they cannot be vertices)

Our algorithm: BRASSENS Relies on Assumptions of Sparsity and Separability for Elegant NMF Solving.

# BRASSENS with sparsity $k = 2$



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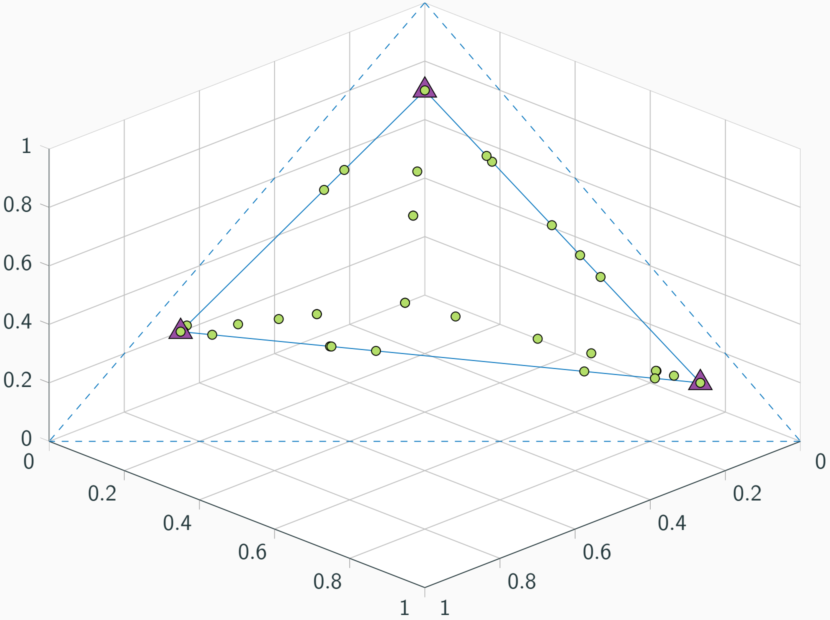

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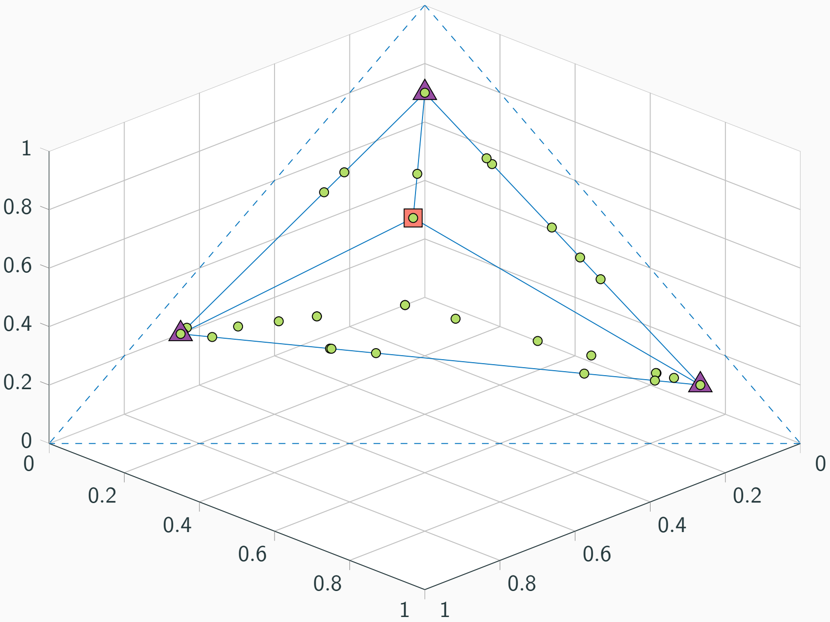

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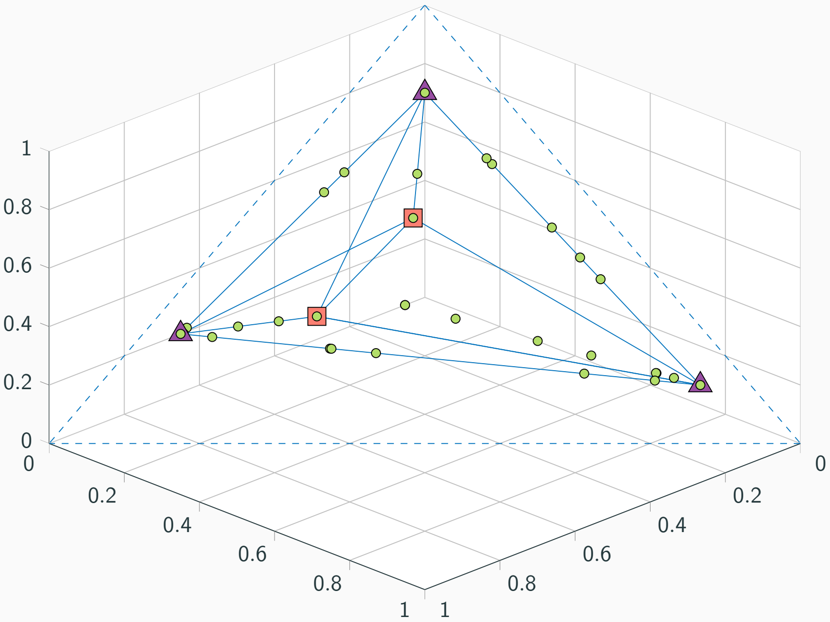

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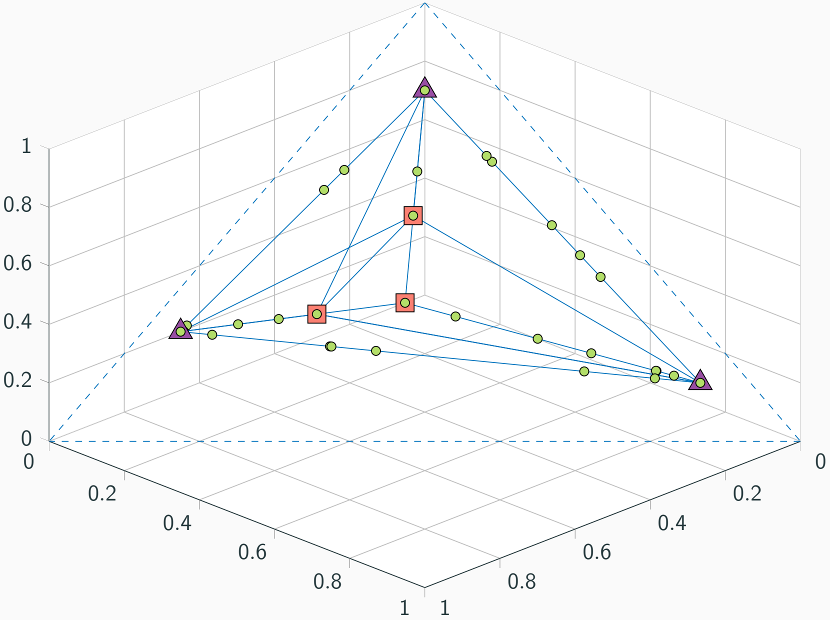

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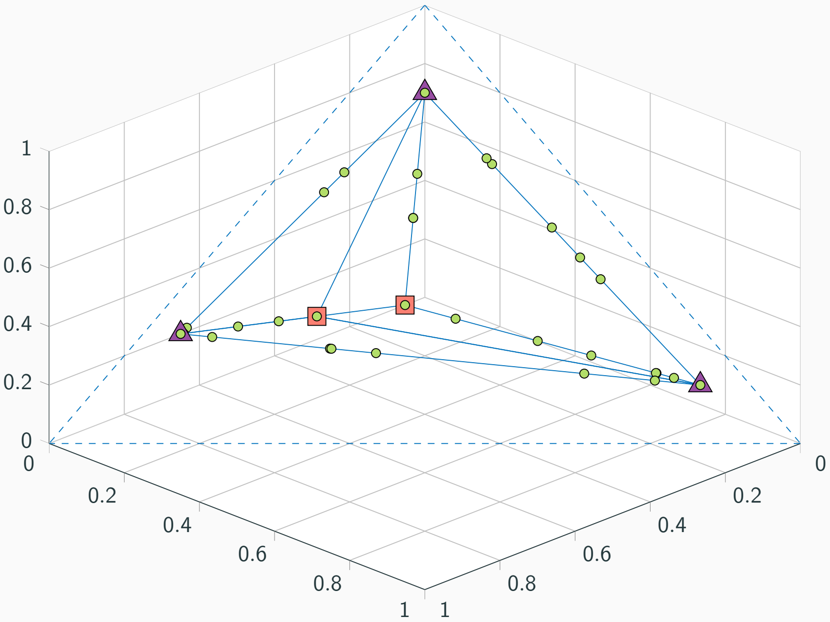

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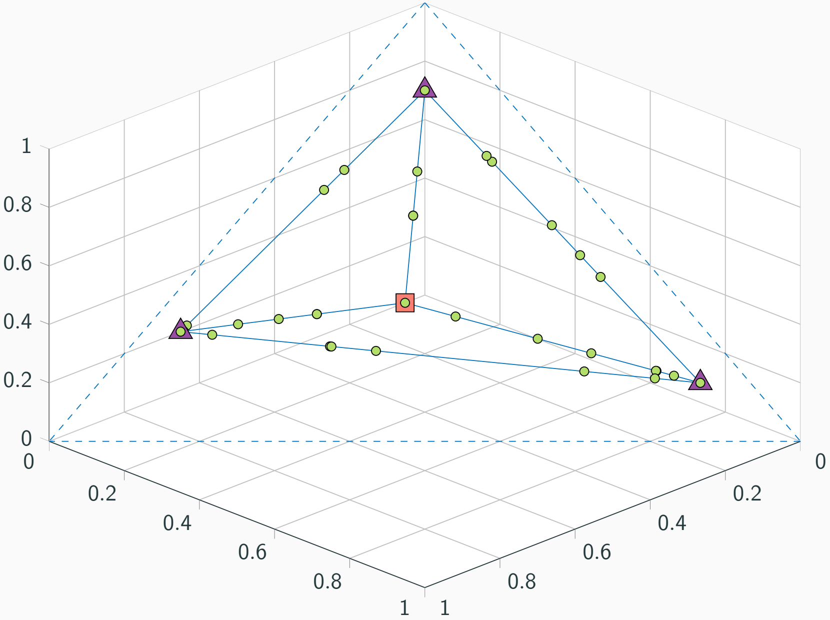


# Complexity

- As opposed to Sep NMF, SSNMF is NP-hard (Arnaud proved it, see the paper)
- Hardness comes from the $k$-sparse projection
- Not too bad when $r$ is small, with our BnB solver

# Correctness

**Assumption 1** No column of W is a nonnegative linear combination of k other columns of W.
$\Rightarrow$ necessary condition for recovery by BRASSENS

**Assumption 2** No column of W is a nonnegative linear combination of k other columns of M.
$\Rightarrow$ sufficient condition for recovery by BRASSENS

If data points are $k$-sparse and generated at random, **Assumption 2** is always true, so **Assumption 1** becomes sufficient.

# Related work

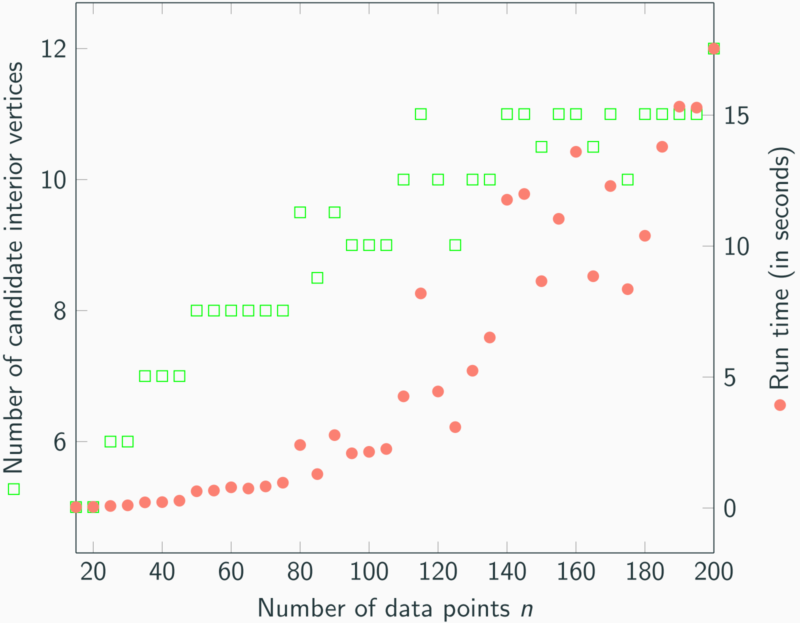
Only one similar work: [Sun and Xin, 2011]

- Handles only one interior vertex
- Non-optimal bruteforce-like method

# Experiments

- Experiments of synthetic datasets with interior points
- Experiment on underdetermined multispectral unmixing (Urban image, $309 \times 309$ pixels, limited to $m = 3$ spectral bands, and we search for $r = 5$ materials)
- No other algorithm can tackle SSNMF, so comparisons are limited

# XP Synthetic 1: number of data points grows



# XP Synthetic 2: dimensions grow

| m | n | r | k | Number of candidates | Run time in seconds |
|---|---|---|---|---|---|
| 3 | 25 | 5 | 2 | 5.5 | 0.26 |
| 4 | 30 | 6 | 3 | 8.5 | 3.30 |
| 5 | 35 | 7 | 4 | 9.5 | 38.71 |
| 6 | 40 | 8 | 5 | 13 | 395.88 |

Conclusion from experiments:

- kSSNPA is efficient to select few candidates
- Still, BRASSENS does not scale well :(

# XP on 3-bands Urban dataset with $r = 5$

SNPA

BRASSENS (finds 1 interior point)

# XP on 3-bands Urban dataset with $r = 5$

Interpretation

| Image | Materials extracted by SNPA | Materials extracted by BRASSENS |
|---|---|---|
| 1 | Grass + trees + roof tops | Grass + trees |
| 2 | Roof tops 1 | Roof tops 1 |
| 3 | Dirt + road + roof tops | Road |
| 4 | Dirt + grass | Roof tops 1 and 2 + road |
| 5 | Roof tops 1 + dirt + road | Dirt + grass |

# Future work

- Theoretical analysis of robustness to noise
- New real-life applications

# Take-home messages

Sparse Separable NMF:

- Combine constraints of separability and $k$-sparsity
- A new way to regularize NMF
- Can handle some cases that Separable NMF cannot
  - Underdetermined case
  - Interior vertices
- Is NP-hard (unlike Sep NMF), but actually "not so hard" for small $r$
- Is provably solved by our approach
- Our solution does not scale well

# References i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**Computing a nonnegative matrix factorization – provably.**
STOC '12.

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**Successive Nonnegative Projection Algorithm for Robust Nonnegative Blind Source Separation.**
*SIAM Journal on Imaging Sciences*, 7(2):1420–1450.

Nadisic, N., Vandaele, A., Gillis, N., and Cohen, J. E. (2020).
**Exact Sparse Nonnegative Least Squares.**
In *ICASSP 2020*, pages 5395 – 5399.

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Sun, Y. and Xin, J. (2011).
**Underdetermined Sparse Blind Source Separation of Nonnegative and Partially Overlapped Data.**
*SIAM Journal on Scientific Computing*, 33(4):2063–2094.

Vavasis, S. A. (2010).
**On the Complexity of Nonnegative Matrix Factorization.**
*SIAM Journal on Optimization*.

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Code and exp.: https://gitlab.com/nnadisic/ssnmf

Slides and paper: http://nicolasnadisic.xyz