Estimation of the regularization parameter of an on-line NMF with minimum volume constraint

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IEEE SENSOR ARRAY AND MULTICHANNEL SIGNAL PROCESSING WORKSHOP

11th July 2018

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Introduction

Developing **real-time** hyperspectral image unmixing methods for industrial applications for controlling and sorting pieces of wood.

→ **On-line** Non-negative Matrix Factorization (NMF):

$$\mathbf{X} \approx \mathbf{S}\mathbf{A}.$$

Sequentially updating the parameters $\mathbf{S}$ and $\mathbf{A}$ as the size of the data matrix $\mathbf{X}$ increases.

→ **On-line MVS-NMF (Minimum Volume Simplex-NMF)** [Nus et al., *SSP '18*].

Introduction

$$\mathscr{J}^{(k+1)}\left(\mathbf{S}^{(k+1)},\mathbf{A}^{(k+1)}\right)=\alpha\sum_{\ell=1}^{k}\left\|\tilde{\mathbf{X}}^{(\ell)}-\tilde{\mathbf{S}}^{(\ell)}\tilde{\mathbf{A}}^{(\ell)}\right\|_F^2+(1-\alpha)\left\|\tilde{\mathbf{X}}^{(k+1)}-\tilde{\mathbf{S}}^{(k+1)}\tilde{\mathbf{A}}^{(k+1)}\right\|_F^2$$
$$+\mu\ln\det\left(\tilde{\mathbf{S}}^{(k+1)T}\tilde{\mathbf{S}}^{(k+1)}\right).$$

- The weighting coefficient α $(0\leq\alpha\leq 1)$ adds some tracking capacity to the algorithm.
- The endmembers vary only slightly between consecutive samples *i.e.* $\tilde{\mathbf{S}}^{(k+1)}\approx\tilde{\mathbf{S}}^{(k)}$ [Bucak and Gunsel, 2009].

→ Estimation of **S** and **A**: minimizing the cost function using a gradient descent technique.
→ The strength of the MVS constraint is controlled by the hyperparameter μ; the main goal is to provide a method to determine it automatically.

Some classical approaches for regularization parameter estimation

- The generalized cross validation method [Golub et al., 1979]. As the NMF problem is bilinear, it is not applicable.
- The L-curve [Hansen, 1992].
  → The optimal value of the hyperparameter: maximum curvature of the L-curve.
  → Multi-objective optimization [Kaufman, 1997].
  → Non-convex and the maximum curvature is not guaranteed to be unique.
- [Belge et al., 2002] proposed the Minimum Distance Criterion (MDC) applied to the L-curve (bi-objective case).
  → Limiting the range of the hyperparameter.
- To overcome these two main drawbacks: MDC on response curve (bi-objective case) defined as the linear plot of regularization cost versus the data fitting [Song et al., 2016].

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Response curve

Reformulate the MVS-NMF algorithm as a bi-objective problem:

- Hyperspectral image (slices $\tilde{\mathbf{X}}^{(k)}$, $k = 1, ..., K$), used to learn the value of μ.
- The value of α and the endmembers number are fixed.
- $\mathbf{S}_\mu^{(K)}$ and $\mathbf{A}_\mu^{(K)}$ denote the estimated endmembers and abundances for a given value of μ.

$$\mathscr{J}_1(\mu) = \mathscr{J}_1(\mathbf{S}_\mu^{(K)}, \mathbf{A}_\mu^{(K)}) = \frac{1}{K}\sum_{k=1}^{K} \left\| \tilde{\mathbf{X}}^{(k)} - \tilde{\mathbf{S}}_\mu^{(k)} \tilde{\mathbf{A}}_\mu^{(k)} \right\|_F^2.$$

$$\mathscr{J}_2(\mu) = \mathscr{J}_2(\mathbf{S}_\mu^{(K)}) = \frac{1}{K}\sum_{k=1}^{K} \det\left(\tilde{\mathbf{S}}_\mu^{(k)T} \tilde{\mathbf{S}}_\mu^{(k)} \right).$$

Response curve

Difficulties of the approach:

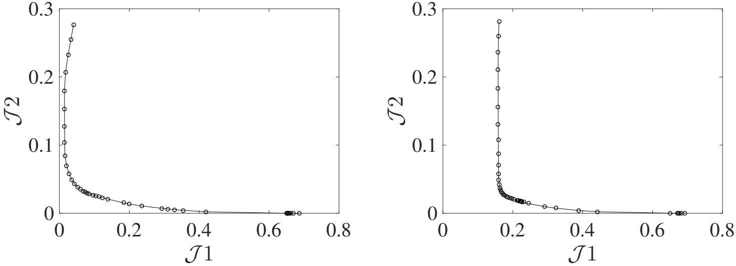
- NMF problems (including MVS-NMF) are bilinear and thus non-convex.
- The obtained solution depends on the initial values of the endmembers and abundances.

What is the shape of a response curve? What is the variability of the response curves for different initial values?

Shape of response curve on a simulated image

- Simulated hyperspectral image consisting in the non-negative mixture of three endmembers, not varying over time.
- None of the three endmembers has any zero value.
  → Decomposition NMF non-unique.
- The three abundance maps are randomly drawn from a continuous uniform distribution on the interval $[0, 1]$.
- The pure pixel condition is approximately fulfilled.
- Noise was added up to have an $SNR = 26dB$.
- $r = 3$ and $\alpha = 0.99$.
- 44 values of $\mu \in [0.0001 \;\; 0.0028]$.

Shape of response curve on a simulated image

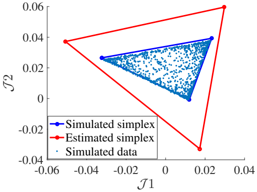


(a) Response curve (noise-free case) (b) Response curve (noisy case)

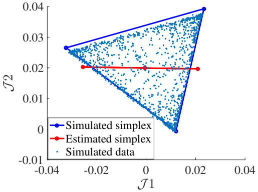
→ The noise is right shifting the response curve by a value which increases with the noise level.

Shape of response curve on a simulated image

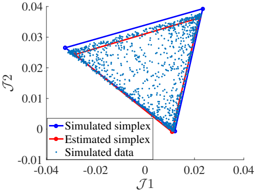
Noisy case



(c) $\mathscr{D} \subset \mathscr{S} (\mu = 0.0001)$

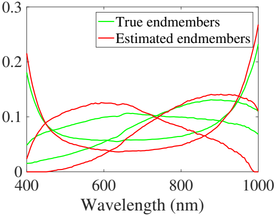


(d) $\mathscr{D} \not\subset \mathscr{S} (\mu = 0.002)$

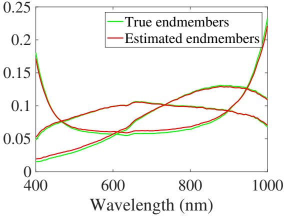


(e) $\mathscr{D} \approx \mathscr{S} (\mu = 0.001)$

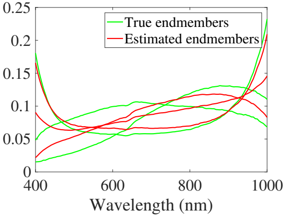
Estimated endmembers for different values of μ



(f) $\mu = 0.0001$



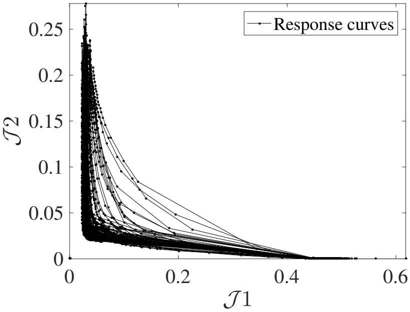
(g) $\mu = 0.001$



(h) $\mu = 0.002$

Influence of the initial conditions

Response curves obtained for 100 different initial values drawn randomly from uniform distribution on the interval $[0, 1]$.



→ Most of the response curves are very similar, but some are deviating from the "mean response curve".

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Three strategies

Estimation of the optimal value of μ. Three strategies are considered:

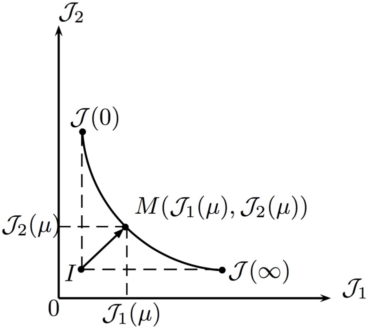
- MDC to the **Pareto Front** estimated from the set of response curves.
- MDC to the **average response curve** to assess how the variability induced by the different initialization is affecting the result.
- MDC to a **single realization** of the response curve.

Pareto Front

- The definition of the Pareto front relies on the notion of domination defined in [Deb, 2001].
- **Non-dominated** or **Pareto optimal** solution: if all other solution in the feasible set has a higher value in at least one of the objectives $\mathscr{J}_i$, with $i \in 1, 2$.
- The image of all the non-dominated solutions is called **Pareto Front**.

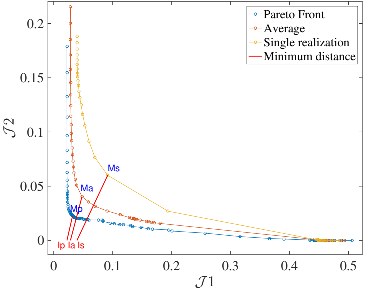
The shape of the Pareto front represents the set of the best achievable tradeoffs between conflicting objectives.

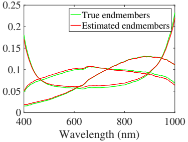
Minimum Distance Criterion



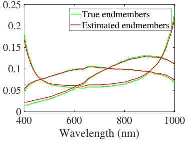
- **The ideal point** I: the point whose coordinates are the minima of the two objective functions.
- **The optimal point** M: the point having the minimum distance to this ideal point.

Results on simulated hyperspectral image



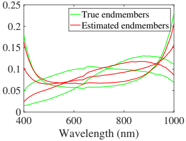


(i) $\mu = 0.00095$



(j) $\mu = 0.0015$

L-curve.

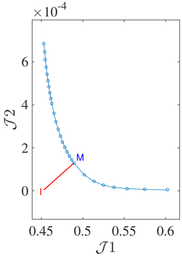


- $\mu = 0.0024$.
- Non-uniqueness.

- Pareto Front: $\mu = 0.00095$.
- Average: $\mu = 0.0011$.
- Single realization: values of μ between 0.001 and 0.0015.

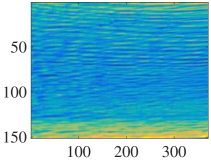
Results on real hyperspectral image

- Single realization strategy.
- Initialization **warm start**.
- 27 values of $\mu \in [0.001 \;\; 0.1]$.

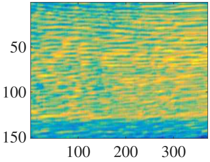


- Value of μ estimated by the MDC: 0.03.

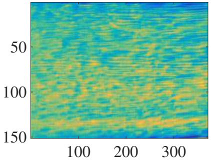
Results on real hyperspectral image



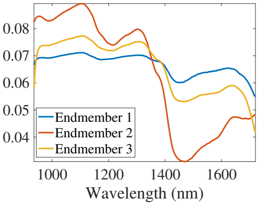
(m) Abundance 1



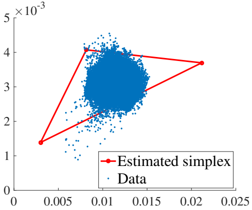
(n) Abundance 2



(o) Abundance 3



(p) Estimated endmembers



(q) Estimated simplex

Limits of the approach for a real hyperspectral image

- Same wood species: oak.
- From one sample to another: the extracted endmembers are very similar and therefore highly correlated.
- Having a "good" initialization: endmembers from an upstream learning.
- Random initialization is complicated: the algorithm converges slowly.

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Conclusions:

- Estimation of the regularization hyperparameter for the on-line MVS-NMF.
- Three different MDC-based strategies: all yielding similar results for a simulated image.
- The single realization response curve approach is the most attractive since it presents the lowest computational cost.
- Validation on a real image using a single realization.
- Possibility to learn the regularization parameter on-line (required for industrial applications).

Perspectives:

- Other volume constraints such as the minimum distance between endmembers. Easier to implement and less sensitive.
- Prove the convexity of response curve that guarantees the uniqueness of the MDC.

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