Sparse BSS in the large-scale regime

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Abstract

Standard Blind Source Separation (BSS) methods allow to efficiently analyze large-scale multichannel data. They nevertheless fail at dealing with problems involving a large number of sources. Building upon standard BSS algorithms, we propose investigating the performances of block-coordinate optimization strategies to handle this case. The use of blocks of intermediate sizes will be shown to yield both a dramatic improvement in the separation quality, which can potentially become perfect up to the numerical errors, and a gain in computation time.

Context

- In BSS, some multichannel data X composed of n row observations are assumed to be the linear combination, entangled of noise N, of k unknown elementary sources Si of t samples: X = AS + N [1].
- Goal: estimate A and S from the sole X, which is an ill-posed unsupervised matrix separation problem.
- Classical methods promote some discriminant information: ICA or its efficient implementation FastICA assumes statistically independent sources [1]. Non-Negative Matrix Factorization (NMF) assumes that the coefficients of A and S are non-negative. We will focus on sparse sources (EFICA, RNA, GMCA [2]...).
- With most algorithms, the separation tends however to deteriorate for large values of n.

Multi-convex optimization and proposed method

A way to perform sparse BSS is to look for a minimizer of:

\[
\min_{A,S} \frac{1}{2} \|X - AS\|^2 + J(A) + G(S)
\]

J(·) and G(·) are used to enforce some constraints on A and S. We studied several cases:

- For \( K \):
  - \( \ell_1 \) sparsity constraint: \( G(S) = \| S \|_1 \)
  - \( \ell_0 \) sparsity constraint in a transformed domain and non-negativity in the direct domain: \( G(S) = \| S \|_0 \| \Phi S \|_1 \)
  - For \( A \):
    - Oblique constraint: \( J(A) = \| A \|_{\infty} \| A \|_{2,\infty} \)
    - Non-negativity and oblique constraint: \( J(A) = \| A \|_{\infty} \| A \|_{2,\infty} + \| A \|_{1,\infty} \)

Multi-convex problem, yielding a determining role to the optimization strategy. So far, blocks [3] of size of 1 (definition or hierarchical methods, e.g. HALS) or n (e.g. GMCA) were used, yielding a trade-off between a less computationally difficult and simpler problem, and error propagations between the estimated sources. This is why we tried an in-between approach: we propose investigating the performances of block-coordinate optimization strategies using blocks of size \( i \in \{1, n\} \).

A two step minimization approach

Our algorithm uses blocks indexed by a set of indices \( I \) of size \( r, 1 \leq r \leq n \).

Warm-up stage: GMCA with blocks [2]

- The results are a first guess used as an input of the PALM stage, which is more sensitive to the initialization and threshold choice.
- Iterative: each update is performed using a projected least-square solution.
- Heuristic approach: decreasing threshold based on GMCA.

PALM algorithm with blocks [4]

- Convergence properties [5].
- Iterative. For each block: a gradient step on the smooth part and a proximal step on the nonsmooth part.
- Use the proximal operators of \( J(·) \) and \( G(·) \): \( \text{prox}_{J(·)} \) and \( \text{prox}_{G(·)} \).

Summary of the algorithm

Warm-up step

For \( k \) from 0 to nmaks:
- Choose a set of indices \( I \)
- Estimation of S with a fixed A: \( S_k^{(0)} = \text{prox}_{J(S)}(X_{k-1}^{(0)}/R_k) \)
- Estimation of A with a fixed \( S_k^{(0)} = \text{prox}_{G(A)}(R_kS_k^{(0)}) \)

Refinement step: initialize with the previous A and S and the corresponding thresholds.

Notwithstanding:
- Choose a set of indices \( I \)
- \( S_k^{(i+1)} = \text{prox}_{J(S)}(X_{k-1}^{(i)}/R_k) \)
- \( A_k^{(i+1)} = \text{prox}_{G(A)}(R_kS_k^{(i+1)} - X_{k-1}^{(i)}) \)

Numerical experiments: simulated matrices

Setting and metric

- A is taken exactly sparse in the direct domain following a Bernoulli-Gaussian distribution.
- A follows a standard normal distribution, has unit columns and a given condition number.
- The metric is computed using the median of \( D = \| \text{PA} \|_2 \| A \|_2 \), where \( \text{A} \) is the true mixing matrix.

Modeling block minimization

- Modelization of the residual as the desired term plus errors:
  \[
  R_k = X - A_k S_k^{(0)} - A_k S_k^{(i+1)} + \epsilon + N
  \]
- The errors can be described in terms of interferences and artifacts \( \epsilon \), being the errors on \( S_k^{(i+1)} \): \( \epsilon' = (A_k^{(i+1)} - A_k^{(0)})^T S_k^{(0)} - \epsilon - \epsilon_k' \)

Trade-off introduced by small blocks: a simpler separation problem vs a larger error.

Numerical experiments: realistic sources

- Simulated LC-1H NMR spectroscopic data of a fluid composed of mixtures of chemical compounds.
- True sources \( S \) but simulated A.
- Sparsity enforced on \( S \) in the wavelet domain and non-negativity for A and \( S \) in the direct domain.

Conclusion and perspectives

The proposed bGMCA algorithm exhibits good performances in comparison to several standard methods, outperforming them in terms of separation quality on many experiments and even reaching perfect separation up to the numerical errors in some cases. The interest of bGMCA is furthermore a dramatic decrease in the computation time, which allows to deal with a large number of sources. To go along with our algorithm, we tried several strategies to choose the blocks.

References