Learning with Low Rank Approximations

or how to use near separability to extract content from structured data

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1. Introduction: separability and matrix/tensor rank

2. Semi-supervised learning: dictionary-based matrix and tensor factorization

3. Complete dictionary learning for blind source separation

4. Joint factorization models: some facts, and the linearly coupled case

Definition: Separability

Let $f : \mathbb{R}^{m_1} \times \mathbb{R}^{m_2} \times \mathbb{R}^{m_3} \to \mathbb{R}$, $m_i \in \mathbb{N}$. Map f is said to be separable if there exist real maps f_1, f_2, f_3 so that

$$f(x, y, z) = f_1(x) f_2(y) f_3(z)$$

Of course, any order (i.e. number of variables) is fine.

Examples:

$(xyz)^n = x^n y^n z^n$, $e^{x+y} = e^x e^y$,
$\int_x \int_y h(x) g(y) dx dy = \left(\int_x h(x) dx\right) \left(\int_y g(y) dy\right)$

Some usual function are not separable, but are written as a few separable ones!

- $\cos(a + b) = \cos(a)\cos(b) - \sin(a)\sin(b)$
- $\log(xy) = \log(x)\mathbb{1}_{y\in\mathbb{R}} + \mathbb{1}_{x\in\mathbb{R}} \log(y)$

A fun case: exponential can be seen as separable for any given order.

Let $y_1(x), y_2(x), \dots, y_n(x)$ s.t. $x = \sum_i^n y_i(x)$ for all $x \in \mathbb{R}$,

$$e^x = \prod_{i=1}^n e^{y_i(x)}$$

Indeed, for any x, setting y_1, y_n as new variables,

$$e^x = e^{y_1+y_2+y_3+\ldots+y_n} := f(y_1, \dots, y_n)$$

Then f is not a separable function of $\sum_i y_i$, but it is a separable function of y_i:

$$f(y_1, y_2, \dots, y_n) = e^{y_1} e^{y_2} \dots e^{y_n} = f_1(y_1) f_2(y_2) \dots f_n(y_n)$$

Conclusion: description of the inputs matters !

Now what about discrete spaces? $(x, y, z) \to \{(x_i, y_j, z_k)\}_{i \in I, j \in J, k \in K}$
$\to$ Values of f are contained in a tensor $\mathcal{T}_{ijk} = f(x_i, y_j, z_k)$.

Example: e^{x_i} is a vector of size I. Let us set $x_i = i$ for $i \in \{0, 1, 2, 3\}$.

$$\begin{bmatrix} e^0 \\ e^1 \\ e^2 \\ e^3 \end{bmatrix} = \begin{bmatrix} e^0 e^0 \\ e^0 e^1 \\ e^2 e^0 \\ e^2 e^1 \end{bmatrix} := \begin{bmatrix} e^0 \\ e^2 \end{bmatrix} \otimes_K \begin{bmatrix} e^0 \\ e^1 \end{bmatrix}$$

Here, this means that a matricized vector of exponential is a rank one matrix.

$$\begin{bmatrix} e^0 & e^1 \\ e^2 & e^3 \end{bmatrix} = \begin{bmatrix} e^0 \\ e^2 \end{bmatrix} \begin{bmatrix} e^0 & e^1 \end{bmatrix}$$

Setting $i = j2^1 + k2^0$, $f(j, k) = e^{2j+k}$ is separable in (j, k).

Conclusion: A rank-one matrix can be seen as a separable function on a grid.

We can also introduce a third-order tensor here:

$$\begin{bmatrix} e^0 \\ e^1 \\ e^2 \\ e^3 \\ e^4 \\ e^5 \\ e^6 \\ e^7 \end{bmatrix} = \begin{bmatrix} e^0e^0e^0 \\ e^0e^0e^1 \\ e^0e^2e^0 \\ e^0e^2e^1 \\ e^4e^0e^0 \\ e^4e^0e^1 \\ e^4e^2e^0 \\ e^4e^2e^1 \end{bmatrix} = \begin{bmatrix} e^0 \\ e^4 \end{bmatrix} \otimes_K \begin{bmatrix} e^0 \\ e^2 \end{bmatrix} \otimes_K \begin{bmatrix} e^0 \\ e^1 \end{bmatrix}$$

By "analogy" with matrices, we say that a tensor is rank-one if it is the discretization of a separable function.

From now on, we identify a function $f(x_i, y_j, z_k)$ with a three-way array $\mathcal{T}_{i,j,k}$.

Definition: rank-one tensor

A tensor $\mathcal{T}_{i,j,k} \in \mathbb{R}^{I \times J \times K}$ is said to be a [decomposable] [separable] [simple] [rank-one] tensor iff there exist $a \in \mathbb{R}^I, b \in \mathbb{R}^J, c \in \mathbb{R}^K$ so that

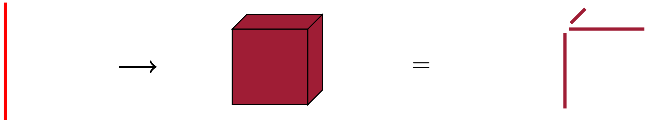
$$\mathcal{T}_{i,j,k} = a_i b_j c_k$$

or equivalently,

$$\mathcal{T} = a \otimes b \otimes c$$

where $\otimes$ is a multiway equivalent of the exterior product $a \otimes b = ab^t$.

What matters in practice may be to find the right description of the inputs !! (i.e. how to build the tensor)



$f(x, y, z, t, \dots)$ $\quad\quad$ $\mathcal{T}$ $\quad = \quad$ $a \otimes b \otimes c$

ALL tensor decomposition models are based on separability

CPD:

$$\boldsymbol{\mathcal{T}} = \sum_{q=1}^{r} a_q \otimes b_q \otimes c_q$$

$$\mathcal{T} = a_1 \otimes b_1 \otimes c_1 + \cdots + a_r \otimes b_r \otimes c_r$$

Tucker:

$$\boldsymbol{\mathcal{T}} = \sum_{q_1,q_2,q_3=1}^{r_1,r_2,r_3} g_{q_1 q_2 q_3} a_{q_1} \otimes b_{q_2} \otimes c_{q_3}$$

Hierarchical decompositions: for another talk, sorry :(

Definition: tensor [CP] rank (also applies for other decompositions)

$$rank(\boldsymbol{\mathcal{T}}) = \min\{r \mid \boldsymbol{\mathcal{T}} = \sum_{q=1}^{r} a_q \otimes b_q \otimes c_q\}$$

Tensor CP rank coincides with matrix “usual” rank! (on board)

If I were in the audience, I would be wondering:

- Why should I care??
  → I will tell you now.
- Even if I cared, I have no idea how to know my data is somehow separable or a low-rank tensor!

  → I don't know, this is the difficult part but at least you may think about separability in the future.

  → It will probably not be low rank, but it may be approximately low rank!

Let $A = [a_1, a_2, \ldots, a_r]$, B and C similarly built.

Uniqueness of the CPD

Under mild conditions

$$krank(A) + krank(B) + krank(C) - 2 \geq 2r, \tag{1}$$

the CPD of $\mathcal{T}$ is essentially unique (i.e.) the rank-one terms are unique.

This means we can interpret the rank-one terms a_q, b_q, c_q
$\rightarrow$ Source Separation!

Compression (also true for other models)

The CPD involves $r(I + J + K - 2)$ parameters, while $\mathcal{T}$ contains IJK entries.

If the rank is small, this means huge compression/dimentionality reduction!

- missing values completion, denoising
- function approximation
- imposing sparse structure to solve other problems (PDE, neural networks, dictionary learning. . .)

- Often, $\mathcal{T} \approx \sum_{q}^{r} a_q \otimes b_q \otimes c_q$ for small r.
- However, the generic rank (i.e. rank of random tensor) is very large.
- Therefore if $\mathcal{T} = \sum_q^r a_q \otimes b_q \otimes c_q + \mathcal{N}$ with $\mathcal{N}$ some small Gaussian noise, it has approximatively rank lower than r but its exact rank is large.

Best low-rank approximate CPD

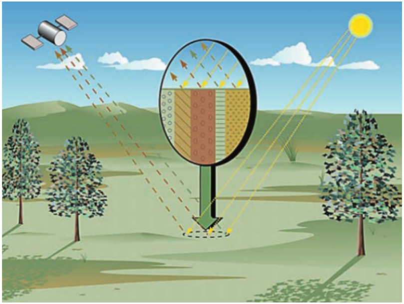
For a given rank r, the cost function

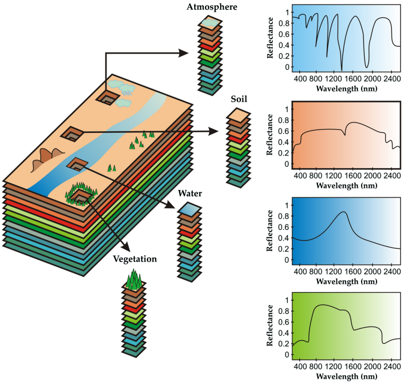
$$\eta(A, B, C) = \|\mathcal{T} - \sum_{q=1}^{r} a_q \otimes b_q \otimes c_q\|_F^2$$

has the following properties:

- it is infinitely differentiable.
- it is non-convex in (A, B, C), but quadratic in A and B and C.
- its minimum may not be attained (ill-posed problem).

My favorite class of algorithms to solve aCPD: block-coordinate descent!





1. Pixels can contain several materials → unmixing!
2. Spectra and Abundances are nonnegative!
3. Few materials, many wavelengths

One material q has separable intensity:

$$I_q(x, y, \lambda) = w_q(\lambda) h_q(x, y)$$

where w_q is a spectrum characteristic to material q, and h_q is its abundance map.

Therefore, for an image M with r materials,

$$I(x, y, \lambda) = \sum_{q=1}^{r} w_q(\lambda) h_q(x, y)$$

This means the measurement matrix $M_{i,j} = \tilde{I}(\text{pixel}_i, \lambda_j)$ is low rank!

Nonnegative matrix factorization

$$\underset{W \geq 0, H \geq 0}{argmin} \|M - \sum_{q=1}^{r} w_q h_q^t\|_F^2$$

where $M_{i,j} = M([x \otimes_K y]_i, \lambda_j)$ is the vectorized hyperspectral image.

Conclusion: I have tensor data, but matrix model! Tensor data $\neq$ Tensor model

1. How to deal with the semi-supervised settings?
   - Dictionary-based CPD [C., Gillis 2017]
   - Multiple Dictionaries [C., Gillis 2018]
2. Blind is hard! E.g., NMF is often not identifiable.
   - Identifiability of Complete Dictionary Learning [C., Gillis 2019]
   - Algorithms with sparse NMF [C., Gillis 2019]
3. What about dealing with several data set (Hyper-Multispectral, time data)?
   - Coupled decompositions with flexible couplings. (Maybe in further discussions)

Semi-supervised Learning with LRA

Nowdays, source separation may not need to be blind!

Hyperspectral images:

- Toy data with ground truth: Urban, Idian Pines...
- Massive ammount of data: AVIRIS NextGen
- Free spectral librairies: ECOSTRESS

How to use the power of blind methods for supervised learning?

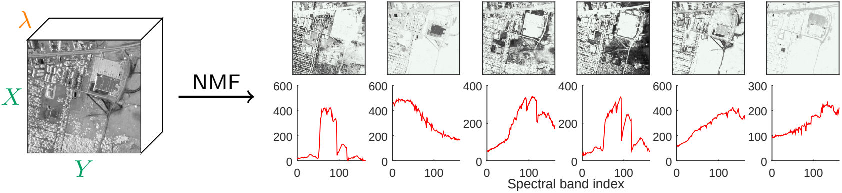
This talk

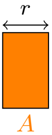
Pre-trained dictionaries are available

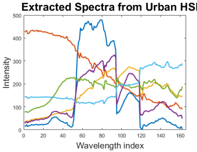
Many other problems (TODO)

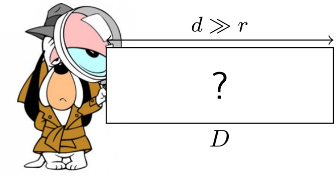
- Test and Training joint factorization.
- Mixing matrix pre-training with domain adaptation.
- Learning with low-rank operators.

Using dictionaries guaranties interpretability

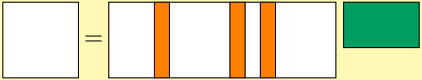








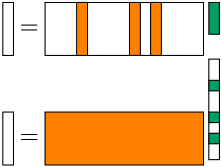
<u>Idea:</u> Impose $A \approx D(:,\mathcal{K})$, $\#\mathcal{K} = R$.



$$M = D(:,\mathcal{K})B$$

1st order model (sparse coding):

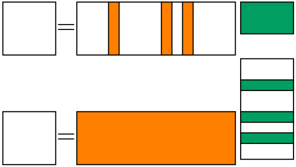
$$\begin{aligned} m &= \sum_{q=1}^{r} \lambda_q d_{s_q} \\ &= D(:,\mathcal{K})\lambda \\ &= D\tilde{\lambda} \end{aligned}$$



for $m \in \mathbb{R}^m$, s_q in $[1, d]$, $\lambda_q \in \mathbb{R}$ and $d_{s_q} \in D$, $\mathcal{K} = \{s_q, q \in [1, r]\}$.

2d order model (collaborative sparse coding):

$$\begin{aligned} M &= \sum_{q=1}^{r} d_{s_q} \otimes b_q \\ &= D(:,\mathcal{K})B \\ &= D\tilde{B} \end{aligned}$$



Tensor 1-sparse coding [C., Gillis 17,18]

$$\mathcal{T} = \sum_{q=1}^{r} d_{s_q} \otimes b_q \otimes c_q$$

- Generalizes easily to any order.
- Alternating algorithms can be adapted easily. Low memory requirement.
- Can be adapted for multiple atom selection (future works).

Theorem: Matrix factorization is identifiable

If $spark(D) \geq r$, $r = rank(M)$, $\#\mathcal{K} = r$, and if there exist $M = D(:, \mathcal{K})B$, then this factorization is unique up to permutations.

Theorem: Tensor factorization is often identifiable

If $spark(D) \geq r$, $r = rank(M)$, $\#\mathcal{K} = r$, and if there exist $\mathcal{T} = \sum_{q=1}^{r} d_{s_q} \otimes b_q \otimes c_q$, then the following holds:

$(B \odot C)$ is full rank $\Rightarrow$ the factorization is unique.

Theorem: 3d order best low-rank approximation exists

If $spark(D) \geq r$, $r = rank(M)$ and $\#\mathcal{K} = r$, then the minimum of

$$\eta(\mathcal{K}, B, C) = \|\mathcal{T} - \sum_{q=1}^{r} d_{s_q} \otimes b_q \otimes c_q\|_F^2$$

always exists.

Earlier results for Multiple Measurements Vectors: [Cotter 05, Chen 06]

$$\underset{A,B,C,\mathcal{K}}{argmin} \quad \|\mathcal{T} - \sum_{q=1}^{r} a_q \otimes b_q \otimes c_q\|_F^2 + \lambda\|\mathbf{A} - \mathbf{D}(:,\mathcal{K})\|_F^2$$

MPALS

Iterate until convergence:
1. Factors are updated by any well-known algorithm (ALS, gradient-based methods. . .).
2. $\mathcal{K}$ is obtained by finding the closest atom in D for each column of A.
3. Increase λ if necessary.

<u>tricks:</u>

- To impose that no atom is selected twice, solve an assignment problem.
- If factors are constrained, simply use any off-the-shelf solver.
- Parameter λ may be tuned for naive flexible dictionary constraint.

$$M = M(:, \mathcal{K})B, \quad B \geq 0$$

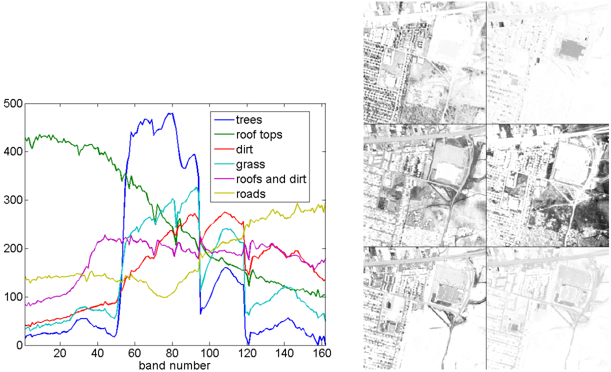
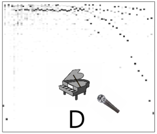
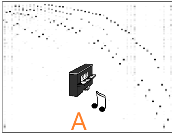


Figure: Spectral signatures and abundance maps identified using MPALS for the Urban data set with $r = 6$.

We badly need more interesting data!

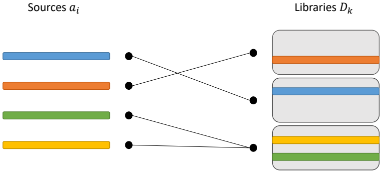
Flexible dictionary constraint: Using known/learnt $p(A|D)$.





Multiple Dictionaries: [C., Gillis 2018]

$A = \Pi[D_1(:, \mathcal{K}_1), \dots, D_N(:, \mathcal{K}_n)], \quad \#\mathcal{K}_i \leq d_i, \quad \sum_i d_i \geq r$

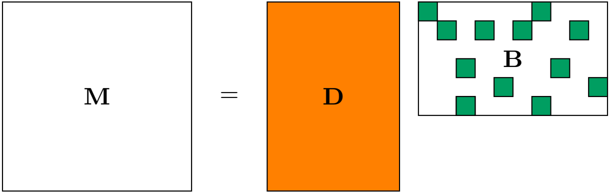


Multiple atoms selection: $A = DS, \quad \|s_i\|_0 \leq k$

Complete Dictionary Learning: Uniqueness and Algorithms with nonnegativity

Given $M \in \mathbb{R}^{d\times n}$ and fixed $r \le d < n$, find $D \in \mathbb{R}^{d\times r}$ and $B \in \mathbb{R}^{r\times n}$ such that

$$\begin{cases} M = DB = \sum_{q=1}^{r} d_q \otimes b_q, \\ \|b_i\|_0 \le k < r, \ \forall i \in [1, n] \end{cases}$$



Problem: Deterministic conditions for the (essential) **uniqueness** of CDL.

<u>other name:</u> Low-rank Sparse Component Analysis

Sparsity may be enough to ensure uniqueness, even with a tractable number of samples!

Theorem (Simplified version)

If each hyperplaned spanned by all but one columns of D contain more than $\frac{r(r-2)}{r-k}$ columns of M with full spark, then CDL is essentially unique.

This implies $\mathcal{O}(\frac{r^3}{(r-k)^2})$ data points are sufficient for ensuring uniqueness.

Tightness: The result is tight if $k = 1$ or $k = r - 1$ or $k = \alpha r$ with fixed $\alpha \in]0, 1[$.

- Contredicts [Georgiev et. al., 2005], see counter examples.
- Improves w.r.t. previously known combinatorial bounds [Aharon 2005].

Or algorithms for k-sparse NMF.

$$\underset{A \geq 0, B \geq 0, \|b_i\|_0 \leq k}{argmin} \|M - \sum_{q=1}^{r} a_q b_q^t\|_F^2$$

Ideas:

1. If k and r are small, trying all $\binom{r}{k}$ zero patterns is tractable.
2. We can try a variant of k-means.

ESNA

1. Update A with fixed H by nonnegative least squares.
2. Update B with fixed W by trying all patterns of zeros (solving $\binom{r}{k}$ nonnegative least squares).

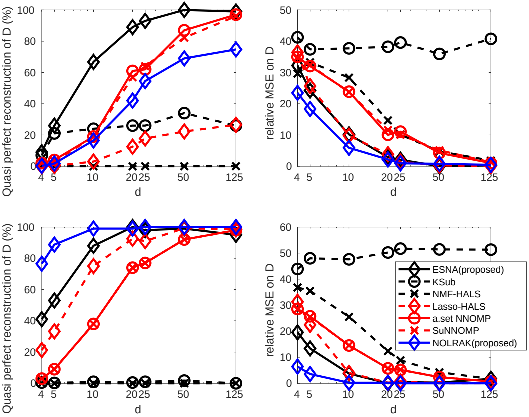
ESNA should (?) be better than any nonnegative sparse coding techniques (NNOMP, Lasso with nonnegativity constraints, ...).

NOLRAK

1. Compute A and B with known zeros in B (averaging step)
2. Compute the zero positions of B (affectation step)

Experimental Setup:

- Goal: Solve exact NDL (identifiable)
- $r = 4$, $k = (2; 3)$, $n = (300; 200)$, $d \in [4, 125]$
- Uniformly sampled D and B, B sparsified to ensure identifiability.
- Results averaged over $N = 100$ trials.



top: $k = 2$; bot: $k = 3$

There is room left for algorithmic improvement!

Also, result on uniqueness of Nonnegative CDL? Overcomplete? Noisy?

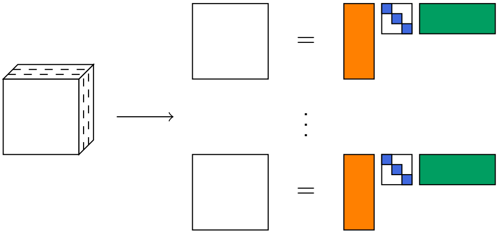
Joint factorization models: some facts, and the linearly coupled case.

$$\mathcal{T} = \sum_{q=1}^{r} a_q \otimes b_q \otimes c_q$$

is equivalent to:

$$M_k = A\Sigma_k B^T = \sum_{q=1}^{r} c_{qk} a_q \otimes b_q$$

with $\mathcal{T}_{::k} = M_k$, $A = [a_1, \ldots, a_r]$, $B = [b_1, \ldots . b_r]$, $\Sigma_k = diag(C_{:k})$



Closing the gap between matrix and tensor factorization: flexible coupling

Several Matrix Factorizations:

$$\forall k \in [1, K],\ M_k = A_k B_k^T$$

Joint Matrix Factorizations = Matrix Factorizations:

$$[M_1, \dots, M_K] = AB^T = A[B_1^T, \dots, B_K^T]$$

$\rightarrow$ same A but different B_k.

Example: Various hyperspectral images with same materials.

Flexible Coupling: linearly coupled factors

For all $k \in [1, K]$,

$$\begin{aligned} M_k &= A \Sigma_k B_k^T \\ 0 &= \mathcal{L}_k(B_k, H) \end{aligned}$$

where $\mathcal{L}_k$ is a bilinear matrix operator and $\mathcal{L}_k(B_k, H) \in \mathbb{R}^{p_3 \times p_4}$, $H \in \mathbb{R}^{p_1 \times p_2}$ for some integers p_i.

$\mathcal{L}_k$ and H can be given, or learned under some structural constraints!

PARAFAC2

$\mathcal{L}_k(B_k, H) := B_k - P_k H$ with $P_k^T P_k = I$ and $P_k \in \mathbb{R}^{J\times r}$ (if $r < J$).

- PARAFAC2 supposes $B_k^T B_k$ is constant.
- P_k can be learnt.
- Constrained version can be difficult to deal with. [C., Bro 2018][Schenker, C., Acar, ongoing work]

Partially coupled factors

$\mathcal{L}_k(B_k, H) = B_k \Sigma_k - H$ where Σ_k is a square diagonal matrix with r_k nonzeros.

By choosing the numbers r_k, one can choose how many components are related in each matrix.

Many models to explore!

Shift PARAFAC [Harshman 2003], Conv PARAFAC [Morup 2008], Registered PARAFAC [C., Cabral-Farias, Rivet 2018]

Separability/LRA + Machine Learning
=
nice research

$f(x,y) = f_1(x)f_2(y)$

Unsupervised Learning or Blind Separation

$M = AB$, $(A,B) \in \mathcal{C}^2$

Structured approximations

$\mathcal{T} = \sum_q^r a_q \otimes b_q \otimes c_q$

Supervised Learning

Neural networks