Joint Tensor Compression for Coupled Canonical Polyadic Decompositions

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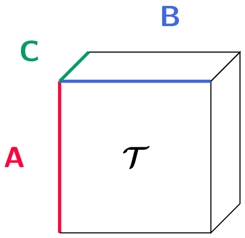
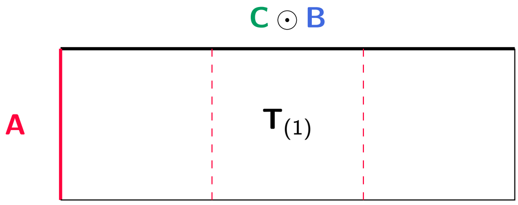
EUSIPCO 2016

Tensor Canonical Polyadic (CP) model



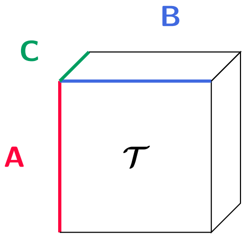
$$\mathcal{T} = (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathcal{I}$$

where $\mathbf{A} \in \mathbb{R}^{I \times R}$ spans the columns of $\mathcal{T}$ unfolded in the 1^{st} mode :



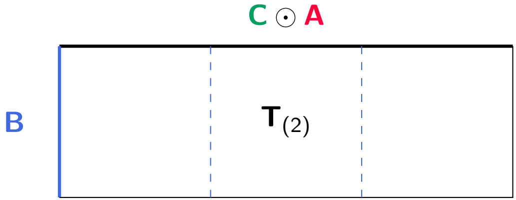
$\in span(\mathbf{A})$

Tensor Canonical Polyadic (CP) model



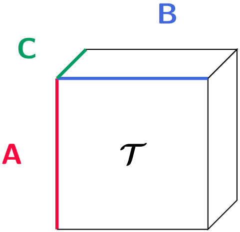
$$\mathcal{T} = (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathcal{I}$$

where $\mathbf{B} \in \mathbb{R}^{J \times R}$ spans the columns of $\mathcal{T}$ unfolded in the 2^{nd} mode :



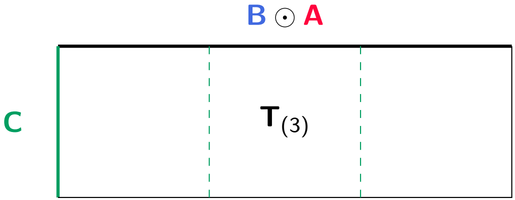
$\in span(\mathbf{B})$

Tensor Canonical Polyadic (CP) model



$$\mathcal{T} = (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathcal{I}$$

where $\mathbf{C} \in \mathbb{R}^{K \times R}$ spans the columns of $\mathcal{T}$ unfolded in the 3rd mode :

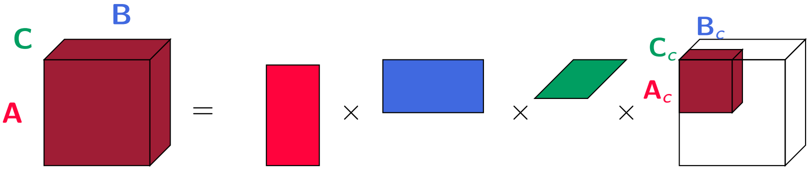


$\in span(\mathbf{C})$

Tensor compression in the noiseless case

Another tensor decomposition : **HOSVD**

$$\mathcal{T} = (\mathbf{U}\mathbf{A}_c \otimes \mathbf{V}\mathbf{B}_c \otimes \mathbf{W}\mathbf{C}_c)\ \mathcal{I}$$



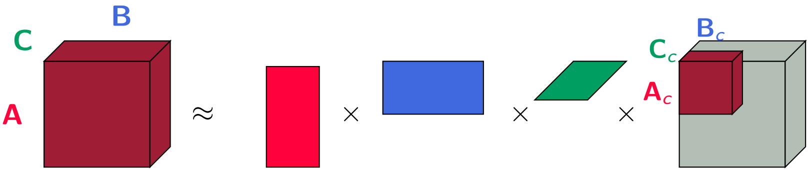
$$\mathcal{T} = (\mathbf{U} \otimes \mathbf{V} \otimes \mathbf{W})\ \mathcal{G}$$

$$\mathcal{G} = (\mathbf{A}_c \otimes \mathbf{B}_c \otimes \mathbf{C}_c)\ \mathcal{I}$$

où $\mathbf{U}\mathbf{N}_1 = SVD(\mathbf{T}_{(1)})$ $\mathbf{V}\mathbf{N}_2 = SVD(\mathbf{T}_{(2)})$ $\mathbf{W}\mathbf{N}_3 = SVD(\mathbf{T}_{(3)})$

Tensor compression in the noisy case

In the noisy case : **truncated HOSVD**



$$\mathcal{T} \approx (\mathbf{U} \otimes \mathbf{V} \otimes \mathbf{W})\,\mathcal{G}$$

où $\hat{\mathbf{U}}\mathbf{N}_1 = TSVD(\mathbf{T}_{(1)})$ $\hat{\mathbf{V}}\mathbf{N}_2 = TSVD(\mathbf{T}_{(2)})$ $\hat{\mathbf{W}}\mathbf{N}_3 = TSVD(\mathbf{T}_{(3)})$

Remark : $\mathbf{C}$ is in the column space of $\mathbf{W}$ but not of $\hat{\mathbf{W}}$!

Tensor CP in the compressed space

$$\widehat{\mathcal{G}} = (\widehat{\mathbf{U}}^\mathsf{T} \otimes \widehat{\mathbf{V}}^\mathsf{T} \otimes \widehat{\mathbf{W}}^\mathsf{T}) \left[(\mathbf{U} \otimes \mathbf{V} \otimes \mathbf{W})(\mathbf{A}_c \otimes \mathbf{B}_c \otimes \mathbf{C}_c)\mathcal{I} + \mathcal{E} \right] =$$
$$(\mathbf{A}_c \otimes \mathbf{B}_c \otimes \mathbf{C}_c)\mathcal{I} + \mathcal{E}_c$$

1. Compress $\mathcal{T}$ using any fast HOSVD
2. Decompose $\widehat{\mathcal{G}}$ to get $\widehat{\mathbf{A}}_c$, $\widehat{\mathbf{B}}_c$, $\widehat{\mathbf{C}}_c$ (ALS for example)
3. Decompress : $\widehat{\mathbf{A}} = \widehat{\mathbf{U}}\widehat{\mathbf{A}}_c$, $\widehat{\mathbf{B}} = \widehat{\mathbf{V}}\widehat{\mathbf{B}}_c$, $\widehat{\mathbf{C}} = \widehat{\mathbf{W}}\widehat{\mathbf{C}}_c$

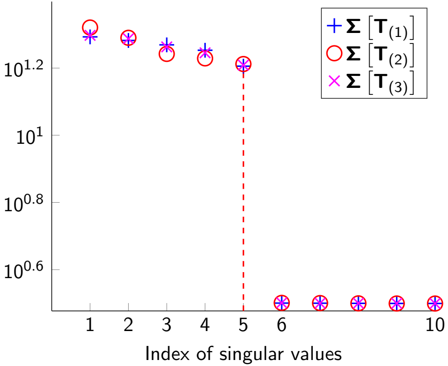
Compressed dimensions : at least tensor rank

Time in seconds for CP dec. $N \times N \times N$ - rank 5 random tensor :

N	10	50	100	200	300
ALS	0.36	0.70	1.92	7.13	26.43
Co-ALS	0.33	0.39	0.45	0.93	2.14

Rank and minimum compressed dimensions

Singular values from the HOSVD in the noisy case ($N = 300$, rank 5)



It suggests **elbow/knee method**

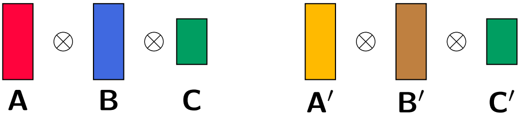
Plan for the rest of the talk

Compression under...

- coupling constraints
- partial coupling constraints
- other coupling constraints

Coupled tensors

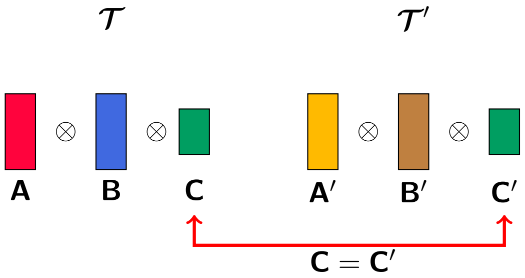
Coupling on 1 factor



Multimodal data fusion

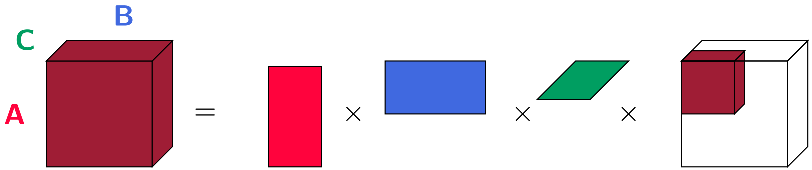
Coupled tensors

Coupling on 1 factor

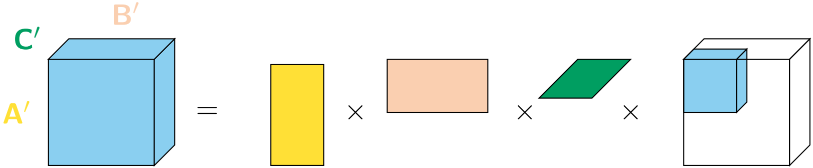


Multimodal data fusion

Joint Compression



$$\mathcal{T}_1 = (\mathbf{U} \otimes \mathbf{V} \otimes \mathbf{W})\,\mathcal{G}$$



$$\mathcal{T}_2 = (\mathbf{U}' \otimes \mathbf{V}' \otimes \mathbf{W}')\,\mathcal{G}'$$

Compression of coupled noisy tensors

$$\mathbf{C} = \mathbf{C}'$$
$$\mathbf{C}_c := \widehat{\mathbf{W}}^T \mathbf{C}$$
$$\mathbf{C}'_c := \widehat{\mathbf{W}}'^T \mathbf{C}'$$

Compression of coupled noisy tensors

$$\mathbf{C} = \mathbf{C}'$$
$$\mathbf{C}_c := \widehat{\mathbf{W}}^T \mathbf{C}$$
$$\mathbf{C}'_c := \widehat{\mathbf{W}}'^T \mathbf{C}'$$
$$\widehat{\mathbf{W}}\mathbf{C}_c \neq \widehat{\mathbf{W}}'\mathbf{C}'_c$$

$\mathbf{C}$ and $\mathbf{C}'$ are not in the column space of $\widehat{\mathbf{W}}$ and $\widehat{\mathbf{W}}'$.

A solution : joint compression

Constrain to have same basis → coupling equality in compressed space !

$$\mathbf{C} = \mathbf{C}'$$

$$\mathbf{C}_c := \widehat{\mathbf{W}}_j^T \mathbf{C}$$

$$\mathbf{C}'_c := \widehat{\mathbf{W}}_j^T \mathbf{C}'$$

A solution : joint compression

Constrain to have same basis → coupling equality in compressed space !

$$\mathbf{C} = \mathbf{C}'$$
$$\mathbf{C}_c := \widehat{\mathbf{W}}_j^T \mathbf{C}$$
$$\mathbf{C}'_c := \widehat{\mathbf{W}}_j^T \mathbf{C}'$$

$$\mathbf{C}_c = \mathbf{C}'_c$$

A solution : joint compression

Constrain to have same basis → coupling equality in compressed space !

$$\mathbf{C} = \mathbf{C}'$$
$$\mathbf{C}_c := \widehat{\mathbf{W}}_j^T \mathbf{C}$$
$$\mathbf{C}'_c := \widehat{\mathbf{W}}_j^T \mathbf{C}'$$

$$\mathbf{C}_c = \mathbf{C}'_c$$

Define $\mathbf{W}_j$ as a basis for stacked 3rd modes $[\mathbf{C}, \mathbf{C}']$:

$$SVD\left(\left[\frac{\mathbf{T}_{(3)}}{\sigma_n}, \frac{\mathbf{T}'_{(3)}}{\sigma'_n}\right]\right) = \widehat{\mathbf{W}}_j \mathbf{N}_j$$

Since same $\mathbf{C}$: **truncate R** columns of $\widehat{\mathbf{W}}_j$

Coupled CP decomposition

Uncompressed problem :

$$\begin{cases} \mathcal{T} = (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathcal{I} + \mathcal{E} \\ \mathcal{T}' = \left(\mathbf{A}' \otimes \mathbf{B}' \otimes \mathbf{C}\right)\mathcal{I} + \mathcal{E}' \end{cases} \quad (1)$$

Compressed problem :

$$\begin{cases} \mathcal{G} = (\mathbf{A}_c \otimes \mathbf{B}_c \otimes \mathbf{C}_c)\mathcal{I} + \mathcal{E}_c \\ \mathcal{G}' = \left(\mathbf{A}'_c \otimes \mathbf{B}'_c \otimes \mathbf{C}_c\right)\mathcal{I} + \mathcal{E}'_c \end{cases} \quad (2)$$

Solve problem (2) with any coupled decomposition algorithm

Application in chemometrics

Fluorescence spectroscopy data :

excitation spectra
emission spectra
mixtures

multimodal chemometrics data set from Acar *et al*[1]

Description

5 compounds : Valine-Tyrosine-Valine (Val), Tryptophan- Glycine (Gly), Phenylalanine (Phe), Maltoheptaose (Mal) and Propanol (Pro)

Nb. of excitation wave lengths	21 (**A**)
Nb. of emission wave lengths	251 (**B**)
Nb. of Mixtures	28 (**C**)
Missing values	30% (replaced by zeros)

1. E. Acar, A.J. Lawaetz, M.A. Rasmussen, and R. Bro. Structure-revealing data fusion model with applications in metabolomics. In Conf. Proc. IEEE Eng. Med. Biol. Soc., pages 6023– 6026. IEEE, 2013

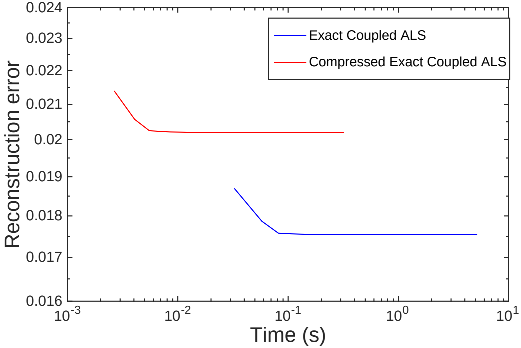
Application in chemometrics

Nuclear magnetic resonance data : chemical shifts
gradient levels
mixtures

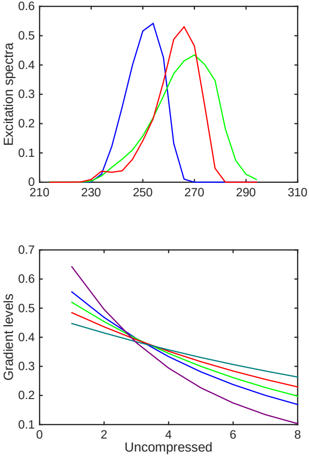
same sample presented previously : **coupling through C**

Nb. of chemical shifts	13324 (**A′**)
Nb. of gradient levels	8 (**B′**)
Nb. of Mixtures	28 (**C**)
Missing values	0% (replaced by zeros)

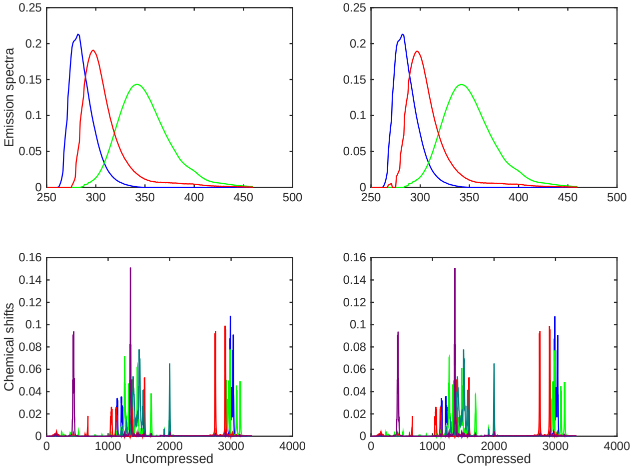
Results


0.024
0.023
0.022
0.021
0.02
0.019
0.018
0.017
0.016
Reconstruction error
10-3
10-2
10-1
100
101
Time (s)
Exact Coupled ALS
Compressed Exact Coupled ALS

Results

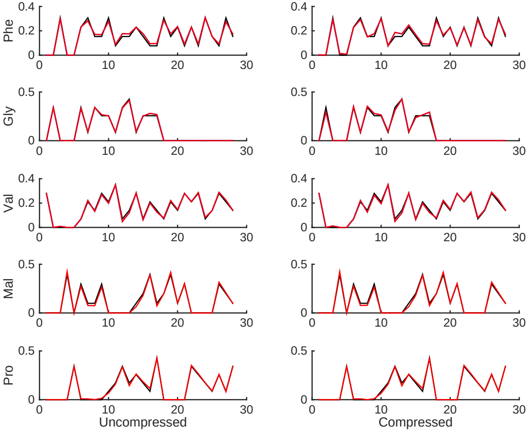

Excitation spectra
0.6
0.5
0.4
0.3
0.2
0.1
0
210
230
250
270
290
310
Gradient levels
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
2
4
6
8
Uncompressed
Compressed

Results



Emission spectra
Chemical shifts
Uncompressed
Compressed

Results



Black lines : ground truth

Partial coupling

Problem : NMR has rank 5, not all components are coupled

Mal and Pro appear in NMR

A solution

For ranks R, R' and R_c coupled components

define $\mathbf{W}_j$ as a basis for stacked 3rd modes $[\mathbf{C}, \mathbf{C}']$:

$$SVD\left(\left[\frac{\mathbf{T}_{(3)}}{\sigma_n}, \frac{\mathbf{T}'_{(3)}}{\sigma'_n}\right]\right) = \widehat{\mathbf{W}}_j \mathbf{N}_j$$

Since same R_c components : **truncate** $\mathbf{R} + \mathbf{R}' - \mathbf{R_c}$ columns of $\widehat{\mathbf{W}}_j$

Partially coupled CP decomposition

Shared components $\mathbf{C}^s$
Unshared components $\mathbf{C}$ and $\mathbf{C}'$

Uncompressed problem :

$$\begin{cases} \mathcal{T} = (\mathbf{A} \otimes \mathbf{B} \otimes [\mathbf{C}^s\,\mathbf{C}])\,\mathcal{I} + \mathcal{E} \\ \mathcal{T}' = \left(\mathbf{A}' \otimes \mathbf{B}' \otimes [\mathbf{C}^s\,\mathbf{C}']\right)\mathcal{I} + \mathcal{E}' \end{cases} \tag{3}$$

Compressed problem :

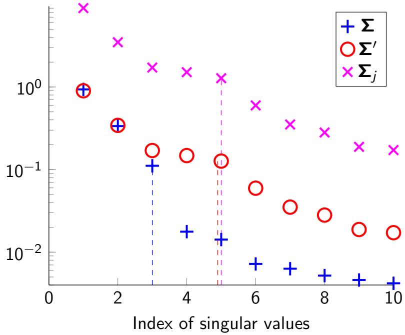
$$\begin{cases} \mathcal{G} = (\mathbf{A}_c \otimes \mathbf{B}_c \otimes [\mathbf{C}_c^s\,\mathbf{C}_c])\,\mathcal{I} + \mathcal{E}_c \\ \mathcal{G}' = \left(\mathbf{A}'_c \otimes \mathbf{B}'_c \otimes [\mathbf{C}_c^s\,\mathbf{C}'_c]\right)\mathcal{I} + \mathcal{E}'_c \end{cases} \tag{4}$$

Ranks and number of coupled components

Exploratory way :

1. R and R' suggested by uncoupled HOSVD
2. R_c from joint SVD of 3rd mode

Elbow/knee of $\boldsymbol{\Sigma}_j$ at $R + R' + R_c$ ($R_c = 3$)



Noisy coupling and Linear coupling

- Noisy coupling

$$\begin{aligned} \mathbf{C} &= \mathbf{C}^{\star} + \mathbf{\Gamma} \\ \mathbf{C}' &= \mathbf{C}^{\star} + \mathbf{\Gamma}' \end{aligned} \tag{5}$$

$$\begin{aligned} \mathcal{T} &= (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C}^{*})\mathcal{I} + (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{\Gamma})\mathcal{I} + \mathcal{E} \\ \mathcal{T}' &= (\mathbf{A}' \otimes \mathbf{B}' \otimes \mathbf{C}^{*})\mathcal{I} + (\mathbf{A}' \otimes \mathbf{B}' \otimes \mathbf{\Gamma}')\mathcal{I} + \mathcal{E}' \end{aligned} \tag{6}$$

- Linear coupling

$$\mathbf{C}' = \mathbf{H}\mathbf{C}, \tag{7}$$

Conclusions

- Compression of CP decomposition : large complexity reduction
  - SVD needs to be fast - Halko *et al* RSVD
  - SVD negligible if multiple initializations needed
- Data fusion setting : joint compression

Perspectives :

- Deal with coupled data of different sizes
- Deal with approximately coupled data

Thank you for your attention !

13th International Conference
on Latent Variable Analysis and Signal Separation

LVA ICA
Grenoble 2017

New submission deadline : Sept. 19th, 2016

Proceedings will be published in Springer LNCS

February 21-23, 2017, Grenoble, France

www.lva-ica-2017.com