Adaptive SP & Machine Intelligence
Multi-way Analysis of Big Data

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Outline

- Challenges in Big Data analytics
- Big Data and Machine Intelligence
- Data structures: From a scalar to a tensor
- Some basic operations on tensors
- Tensorisation $\looparrowright$ a key step in tensor decompositions
- Canonical Polyadic Decomposition (CPD) and its applications
- Links between the CPD and Tucker decomposition
- Partial Least Squares (PLS) and Higher-Order PLS (HOPLS)
- Applications

Big data processing $\looparrowright$ current status

- Computers excel at algorithmic tasks (well-posed mathematical problems)
- Biological systems are superior to digital systems for ill-posed problems with noisy data
- Pigeon: $\sim 10^9$ neurons, cycle time $\sim$ 0.1 seconds. Each neuron sends 2 bits to $\sim$ 1,000 other neurons. This is equivalent to 2×10^{13} bit operations per second
- Old PC: $\sim 10^7$ gates, cycle time 10^{-7} seconds, connectivity $= 2$ $\looparrowright 10 \times 10^{14}$ bit operations per second
- Both have similar raw processing capability, but pigeons are better at recognition tasks
- Is there a way to present large date streams to computers in a more physically meaningful manner?

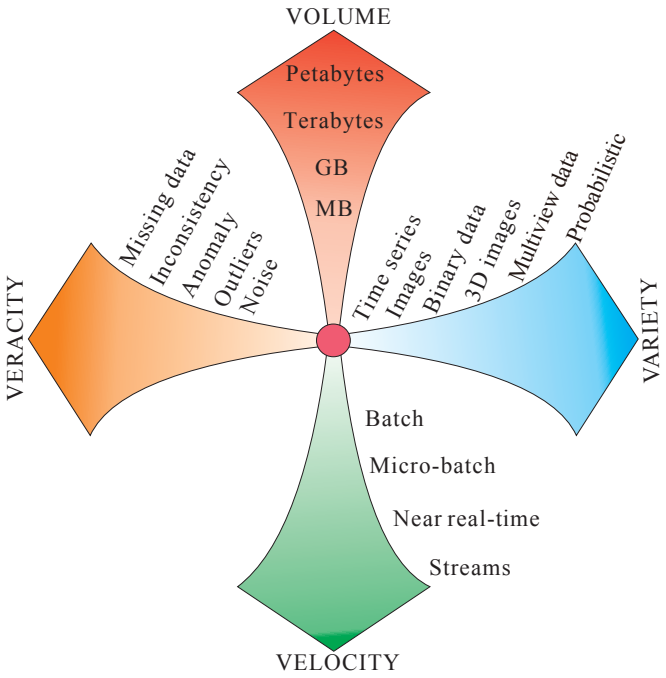
Some facts about Big Data opportunities

According to McKinsey Global Institute, "Big Data: The next frontier for innovation, competition, and productivity", May 2011:

- It would cost USD 600 to by a disk drive which can store all off the music in the world
- In 2010, there were 4 billion mobile phone users in the world
- There is more than 30 billion pieces of content shared on social networks every month
- There is a predicted 40 % growth in global data generated per year versus a 5 % growth in global IT spending
- This all tells us that there are big opportunities for us working in Adaptive Signal Processing and Machine Intelligence

The four V's of big data: Volume, Variety, Velocity, Veracity

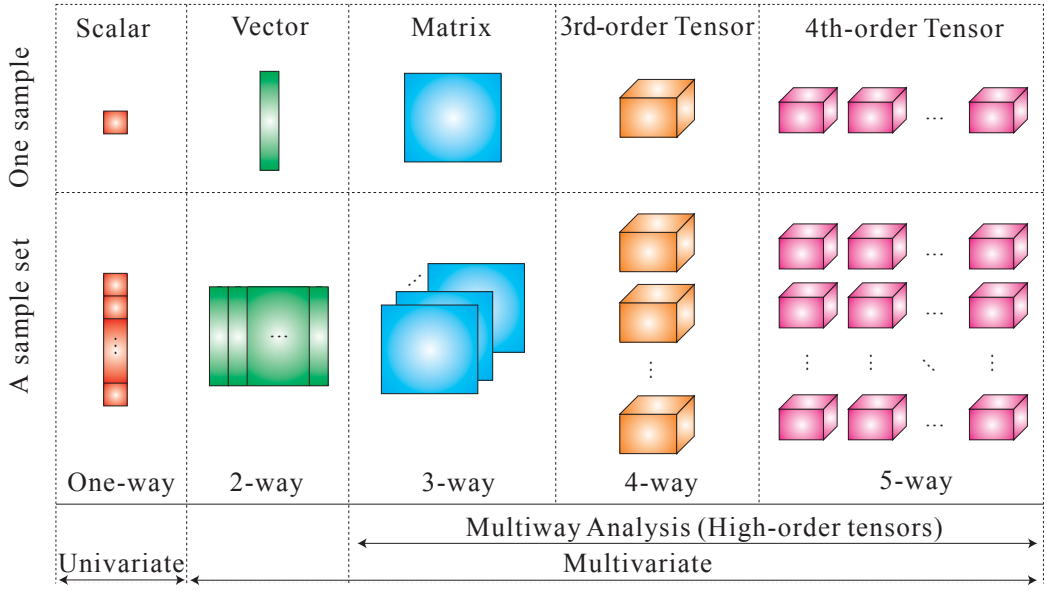
Other V's may include Visualisation, Variability, Value (quality of data), ...



Signal processing an machine learning for big data

Challenges and opportunities

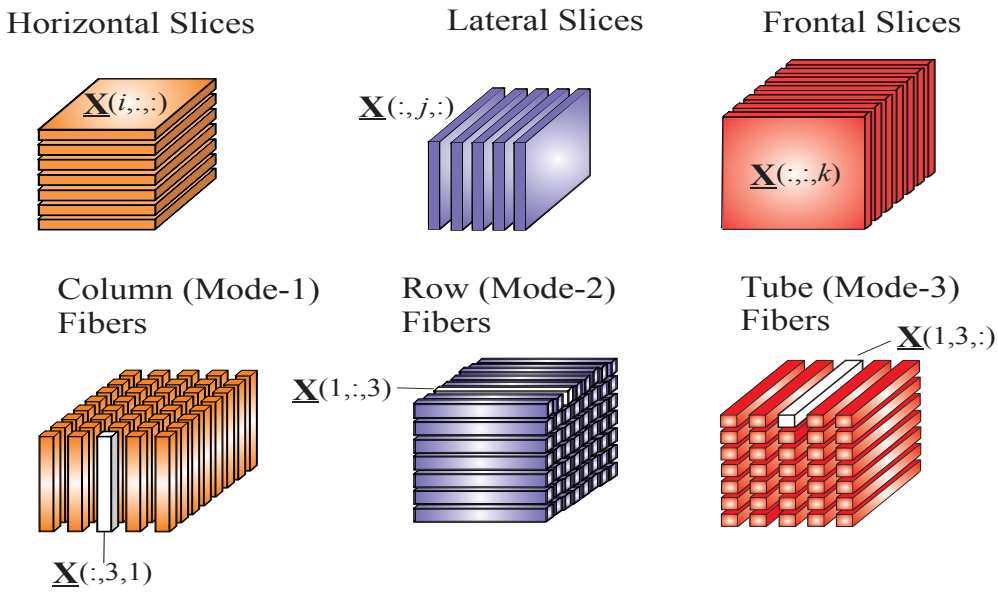
Types of data: From a scalar to a tensor



For example, a 4th-order tensor is a vector of 3rd-order tensors (top right)

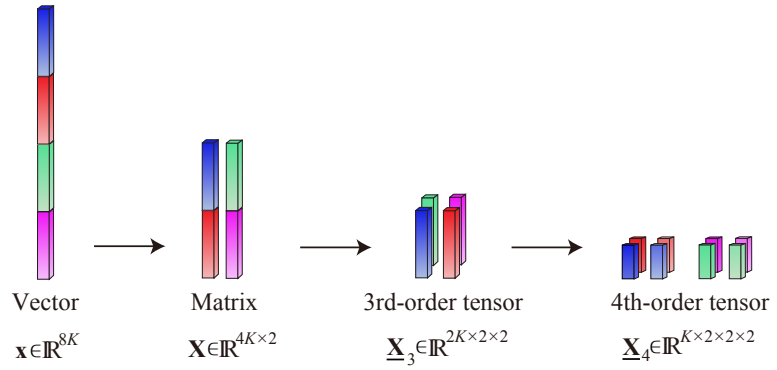
Sub-structures within tensors

order-1 tensor = a vector order-2 tensor = a matrix dimensions = modes



☞ a fiber is produced by fixing two indices and varying one, e.g. $\underline{\mathbf{X}}(1,3,:)$

Tensorisation ↬ blessing of dimensionality

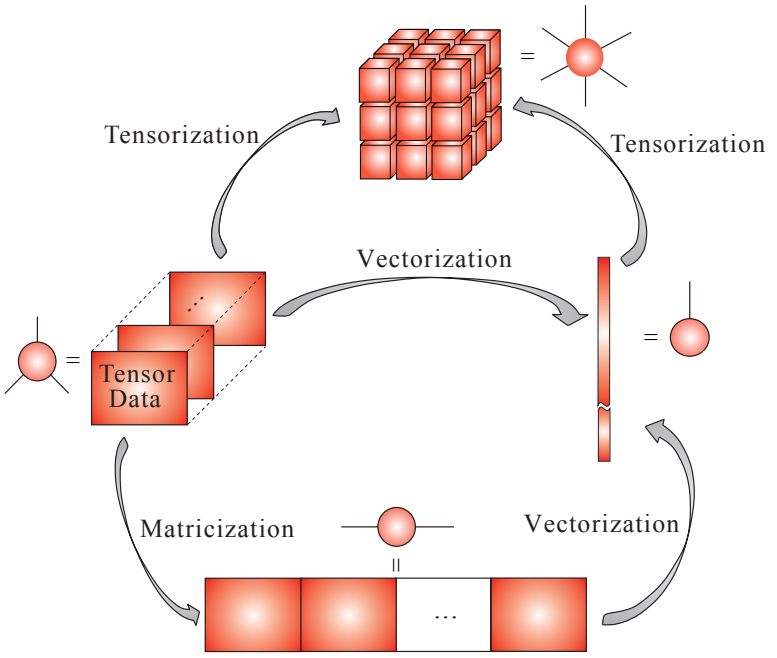


Tensorization (creation of a tensor from a vector of a matrix) can be performed through:

- **Re-arrangement of lower-dimensional data.** One-way exponential sig. $x(k) = az^k$ can be folded into a rank-1 Hankel matrix, thus introducing redundancy (Slide 22)
- **Mathematical construction**. Through e.g. time x frequency x channel representation
- **Experimental design.** EEG data over I channels, J subjects, K trials (Slides 18-21)
- **Natural tensor data.** In HDTV, RGB color images are generated as 3rd-order tensors of size $1920 \times 1080 \times 3$. Similar situation exists in hyperspectral imaging (Slide 35)

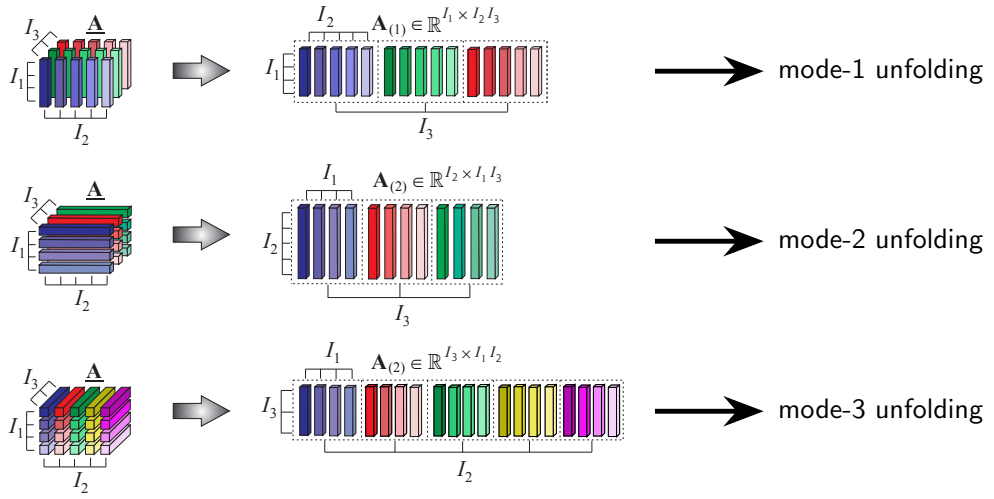
Reshaping of data structures: General concept

Vector, matrix or small-scale tensor ↬ higher-order tensor is referred to as **folding**



Unfolding of a tensor in different modes

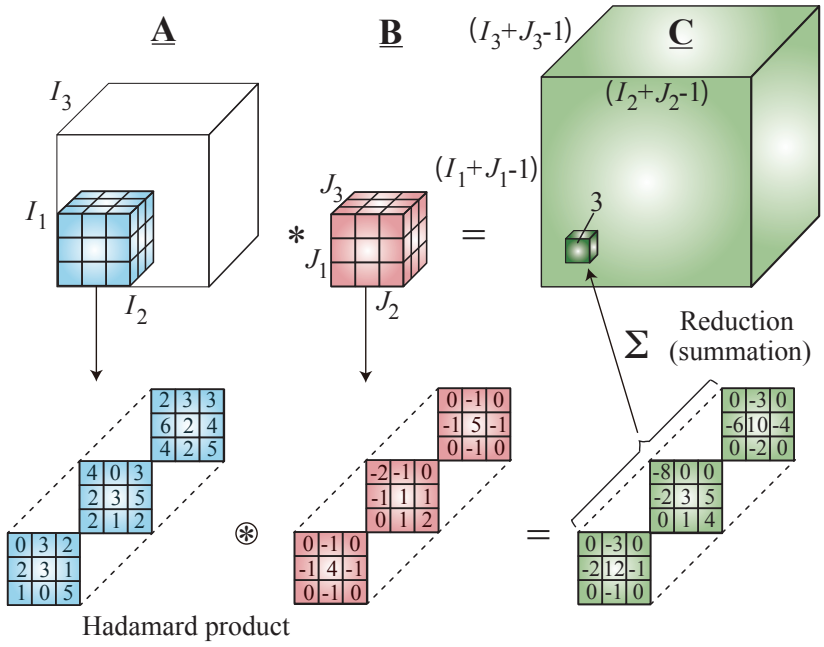
Converts a higher-order tensor into a smaller tensor, matrix, or vector



- This operation maps tensor entries into a matrix, in e.g. a 'slice-by-slice' manner
- Such flattening (unfolding) prior to data analysis breaks the inherent structure in data and obscures latent dependencies between the modes

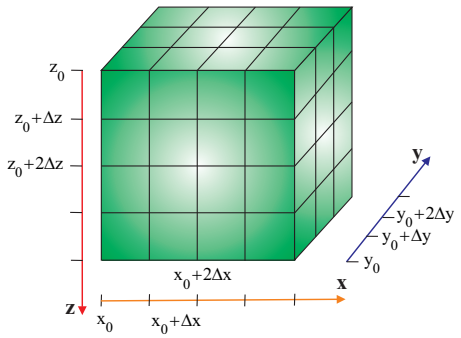
Example 1: Connection with 'flat' DSP, 3D convolution

Many standard operators are readily generalisable to tensors, e.g. the convolution



Curse of dimensionality

- The term **curse of dimensionality** was coined by Bellman (1961) to indicate that the number of samples needed to estimate an arbitrary function with a given level of accuracy grows exponentially with the number of variables, that is, with the dimensionality of the function
- In other words, curse of dimensionality refers to an exponentially increasing number of parameters required to describe an extremely large number of degrees of freedom
- In the context of tensors, the number of elements I^N of an Nth-order tensor of size $I \times I \times \cdots \times I$ grows exponentially with the tensor order, N



Example: Scientific computing

For computational purposes we often need to sample a multidimensional function on a grid (e.g. brain scans)

- For a tri-variate function (N=3, left) sampled at I=1000 points, this will give $I^N = 1000^3 = 10^9$ samples
- For N=4 and I=10,000 this gives $I^4 = 10^{16}$ samples

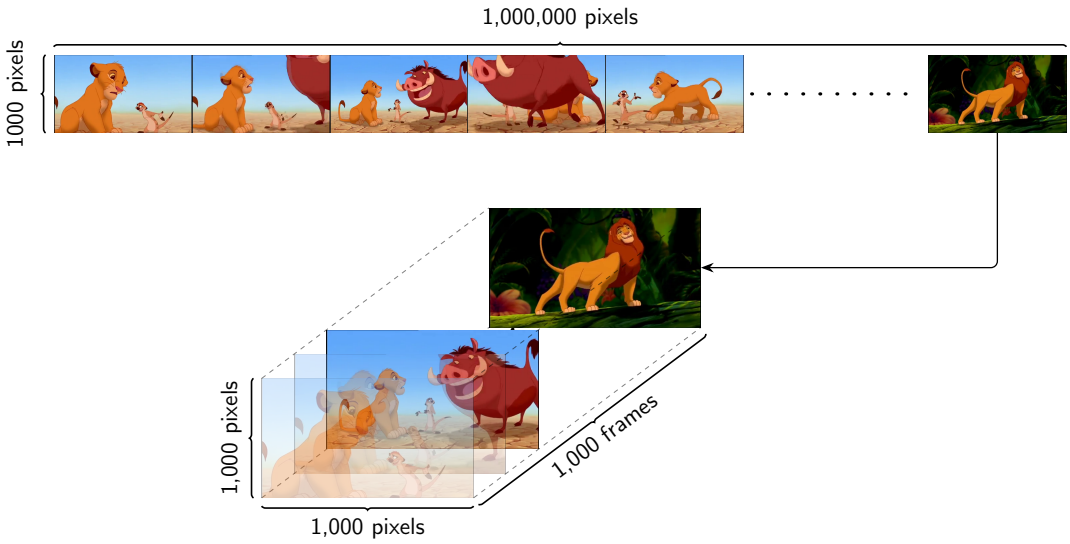
Example 2: From a matrix to a 3D array
Example of a video clip

Each frame is 1,000 pixels by 1,000 pixels $\mathbf{X}_i \in \mathbb{R}^{1,000 \times 1,000}$

20 seconds of recording with 50 FPS rate = 1,000 frames

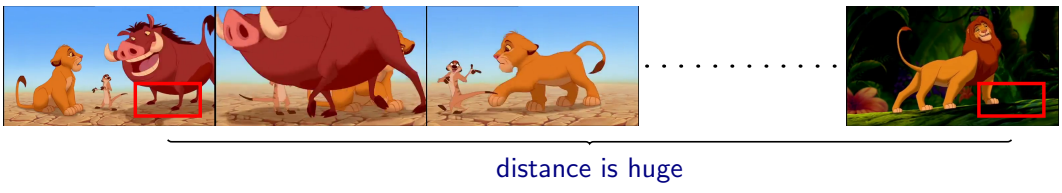
- A video clip can be represented as short and wide matrix $\mathbf{X} \in \mathbb{R}^{1,000 \times 1,000,000}$
- Analysis of all frames at once in this way is not informative or compact
- Significant difference in dimensions ↬ processing is computationally expensive, difficult and not intuitive
- Any PCA-type solution would require a matrix of size $10^6 \times 10^6$
- Visual difference between any two subsequent frames is very small ↬ most information (columns) are redundant
- The most dynamically changing area is the central region. Thus, slight changes at the side of each frame can be almost neglected during most of the analysis
- This is a perfect scenario for low-rank tensor approximations and the inherent super-compression capability of tensor representations
- Why not reshape this awkward-to-analyse data into a compact 3D array?

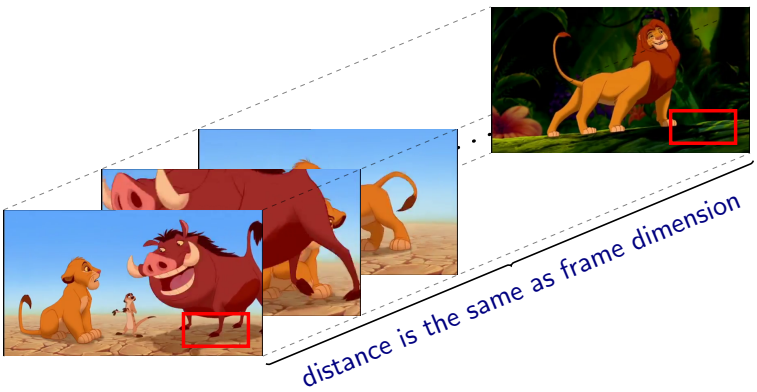
Example 2: Video clip ↬ tensor construction



- A simple re-arrangement of frames (stacking into a cube) transforms the matrix of 1,000 × 1,000,000 pixels into a 3-way tensor of size 1,000 × 1,000 × 1,000

Example 2: Video clip ↬ compact tensor representation

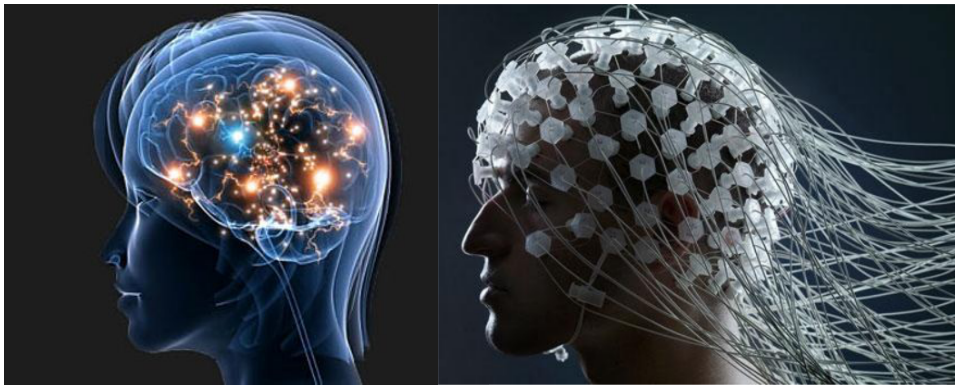




As compared to a matrix case (top row), we have the same number of data points $1000 \times 1000 \times 1000$, but arranged in a much more informative way. This provides a more intuitive and compact data representation and better statistical inference.

Tensorisation: Multi-way representation of multichannel biomedical data

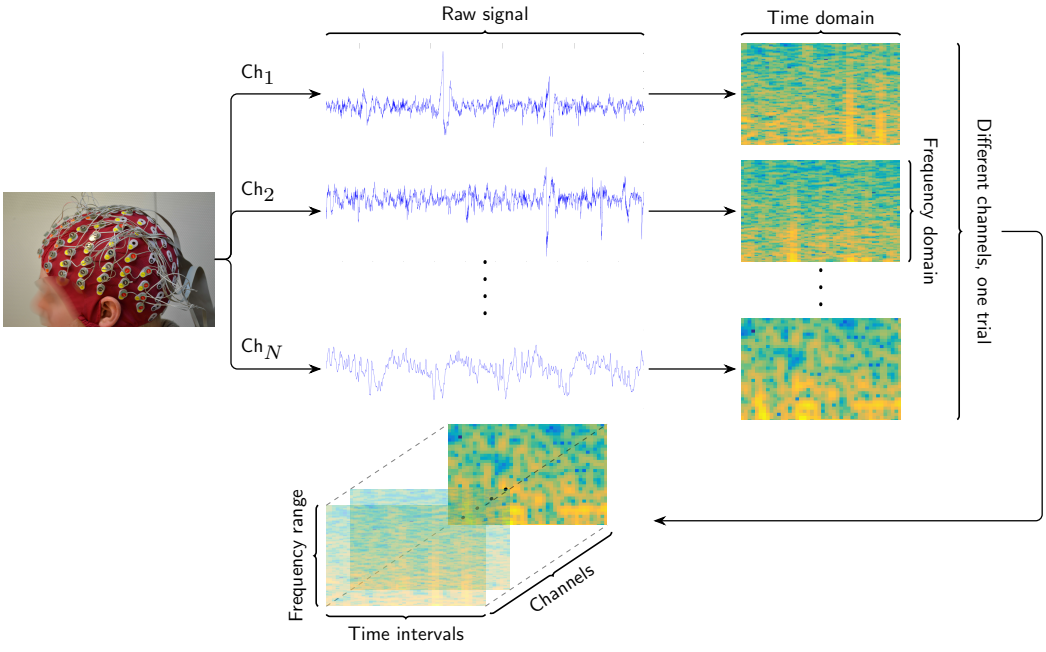
Sources: www.taringa.net and www.hocrox.com



- The electroencephalogram (EEG) is one of the fundamental tools for functional brain imaging, as it is non-invasive and has high temporal resolution
- Brain signals contain latent features which are much more likely to be found from recordings across a large number of recording channels, multiple trials, multiple subjects, multiple stimuli, ...
- The EEG recordings are inherently multi-dimensional (many channels), and multi-way

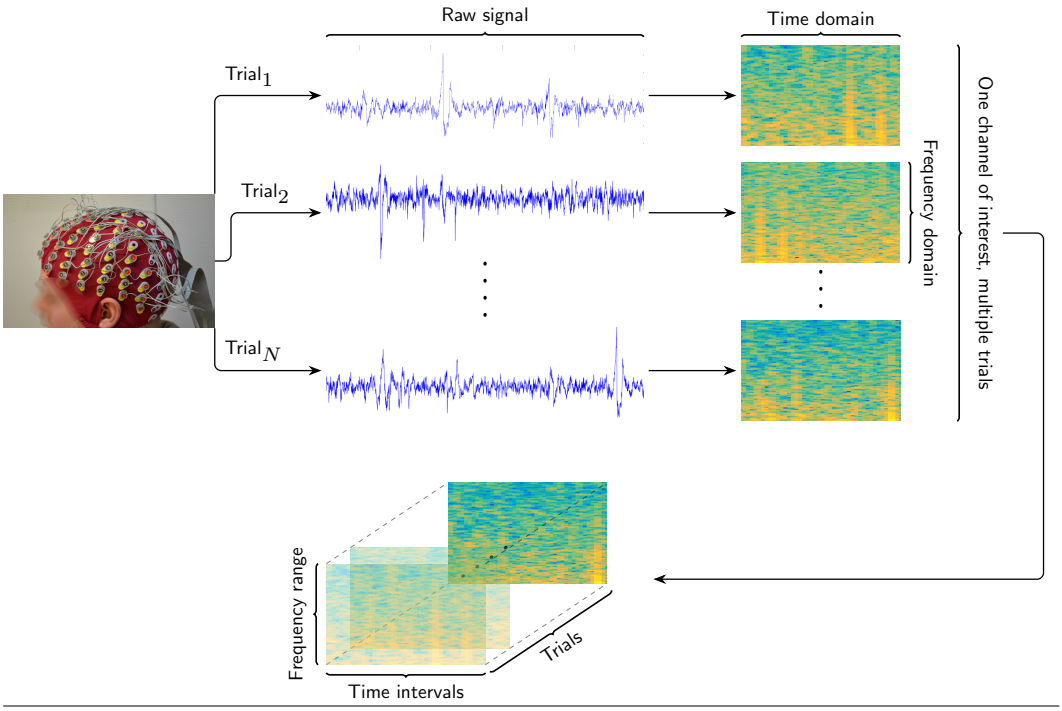
Example 3: Tensor construction from different channels

↪ channel × frequency × time



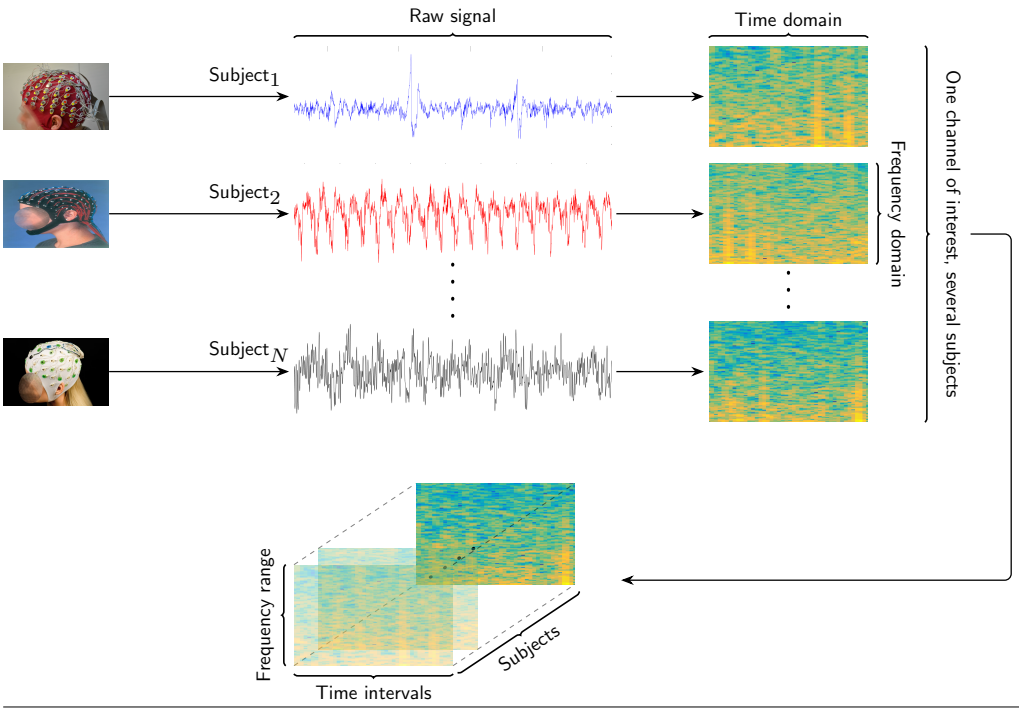
Example 3: Tensor construction from different trials

↪ trial × frequency × time

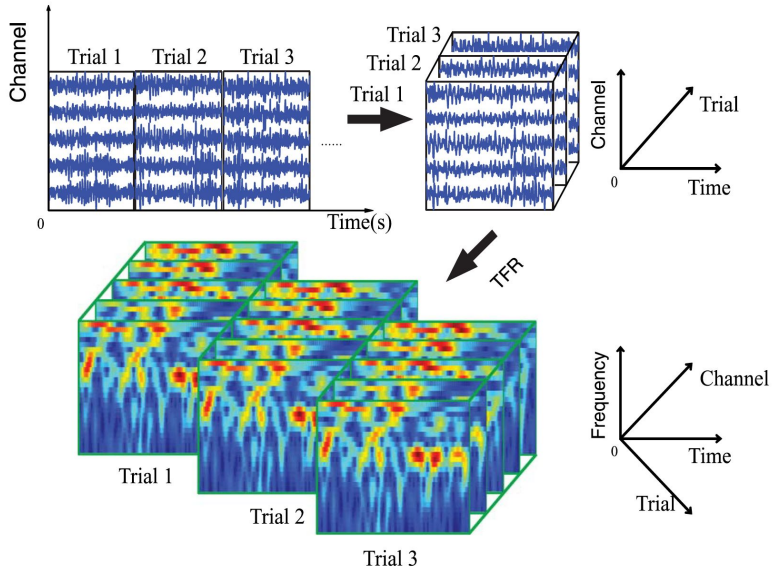


Example 3: Tensor construction from different subjects

↪ subject × frequency × time

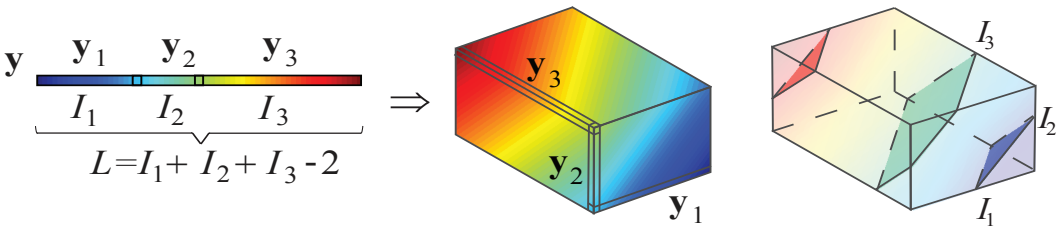


Example 3: Putting it all together ↪ construction of 4D tensor channel × trial × frequency × time



- Each data channel is a matrix of channels × time. Multiple trials form a 3D array
- Time frequency representation (TFR) yields a 4D multi-way array of data. If we include the # Subject, then we have a 5th-order tensor, and so on

Deterministic folding techniques for structured data: The Hankel folding operator



- Consider a sampled exponential signal $\mathbf{z}[k] = az^k$, which produces a data stream

$$\begin{bmatrix} a & az & az^2 & az^3 & \cdots \end{bmatrix} \tag{1}$$

- It can be re-arranged into a Hankel matrix, $\mathbf{H}$, of rank-1 as follows:

$$\mathbf{H} = \begin{bmatrix} a & az & az^2 & \cdots \\ az & az^2 & az^3 & \cdots \\ az^2 & az^3 & az^4 & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix} = a \begin{bmatrix} 1 \\ z \\ z^2 \\ \vdots \end{bmatrix} \begin{bmatrix} 1 & z & z^2 & \cdots \end{bmatrix} = a\, \mathbf{z} \circ \mathbf{z} \tag{2}$$

- For multivariate data, each data channel, i, can be mapped into a Hankel matrix, $\mathbf{H}_i$
- These channel-wise Hankel matrices can then be stacked together into a tensor $\underline{\mathbf{H}}$

Deterministic folding techniques for structured data: The Toeplitz folding operator

- Consider the discrete convolution $\mathbf{z} = \mathbf{x} * \mathbf{y}$ of two vectors, $\mathbf{x}$ and $\mathbf{y}$, of respective lengths I and L >

$$\mathbf{z} = \mathbf{x} * \mathbf{y} \tag{3}$$

- The entries $\mathbf{z}_{I:L}$ can be represented in a linear algebraic form as

$$\mathbf{z}_{I:L} = \mathbf{Y}^T\mathbf{x} = \begin{bmatrix} y(I) & y(I-1) & y(I-2) & \cdots & y(1) \\ y(I+1) & y(I) & y(I-1) & \cdots & y(2) \\ y(I+2) & y(I+1) & y(I) & \cdots & y(3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y(L) & y(L-1) & y(L-2) & \cdots & y(J) \end{bmatrix} \begin{bmatrix} x(1) \\ x(2) \\ x(3) \\ \vdots \\ x(I) \end{bmatrix} \tag{4}$$

- A linear matrix operator, $\mathbf{Y}$, is called the Toeplitz matrix of the generating vector $\mathbf{y}$
- The convolution of three or more vectors allows us to construct a higher-order tensor

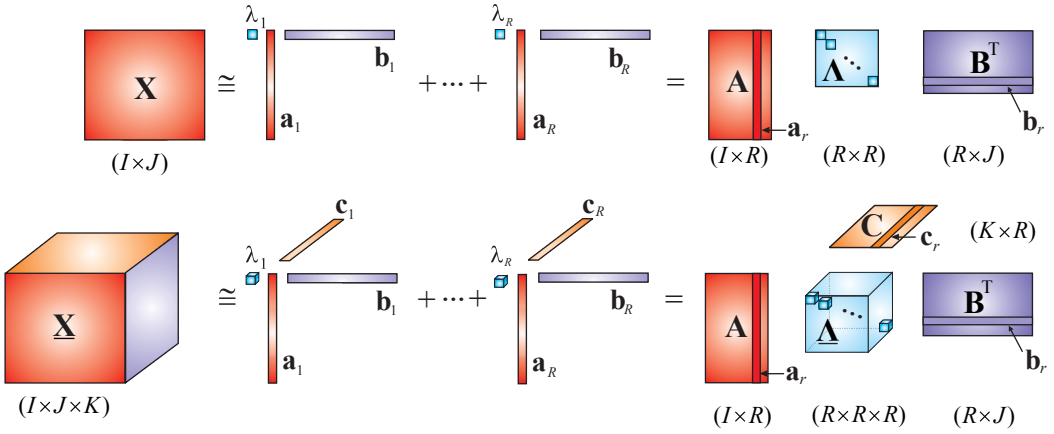
$$\mathbf{z} = \mathbf{x}_1 * \mathbf{x}_2 * \mathbf{y} \tag{5}$$

- First, a Toeplitz matrix $\mathbf{Y}$ is obtained from $\mathbf{x}_1 * \mathbf{x}_2$ as shown in Eq. (4)
- Each row of $\mathbf{Y}(k,:)$, when convolved with a generating vector $\mathbf{y}$, produces its own Toeplitz matrix $\mathbf{Y}_k, k = 1, \ldots, J$
- Finally, stacking all $\mathbf{Y}_k$ along e.g. the third mode, gives the tensor $\underline{\mathbf{Y}} = [\mathbf{Y}_1, \ldots, \mathbf{Y}_J]$

Generalization of Singular Value Decomposition

Top: Singular Value Decomposition (SVD) for matrices

Bottom: Canonical Polyadic Decomposition (CPD) for tensors ↬ tensor rank = R



- Top: A 'flat-view' matrix $\mathbf{X}$ can be decomposed into a sum of rank-1 matrices $\mathbf{X}_i$
- An 3rd-order tensor $\underline{\mathbf{X}}$ captures 3 dimensions (modes) and can be factorised in the same way ↬ as sum of rank-1 tensors $\underline{\mathbf{X}}_i = \mathbf{a}_i \circ \mathbf{b}_i \circ \mathbf{c}_i, i = 1, 2, \ldots, R$
- This is procedure is referred to as the **Canonical Polyadic Decomposition.**
  Canonical ☞ the minimal (rank-1) structure (minimum number of factors).
  Polyadic ☞ the structure is formed by N elements (outer product of N vectors)

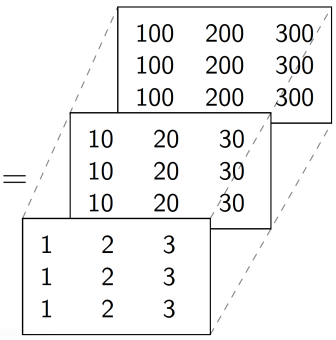
Example 4: The outer product in three dimensions

Consider the vectors $\mathbf{a} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T, \mathbf{b} = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}^T, \mathbf{c} = \begin{bmatrix} 1 & 10 & 100 \end{bmatrix}^T$.

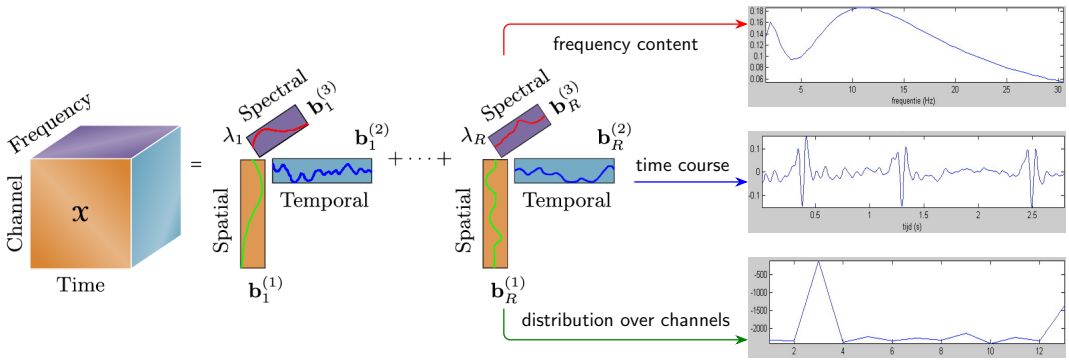
$$\mathbf{a} \circ \mathbf{b} \circ \mathbf{c} = \text{?} \tag{6}$$

$$\mathbf{a} \circ \mathbf{b} \circ \mathbf{c} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \circ \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \circ \begin{bmatrix} 1 \\ 10 \\ 100 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \circ \begin{bmatrix} 1 \\ 10 \\ 100 \end{bmatrix} =$$



Intuition and physical meaning behind the CPD



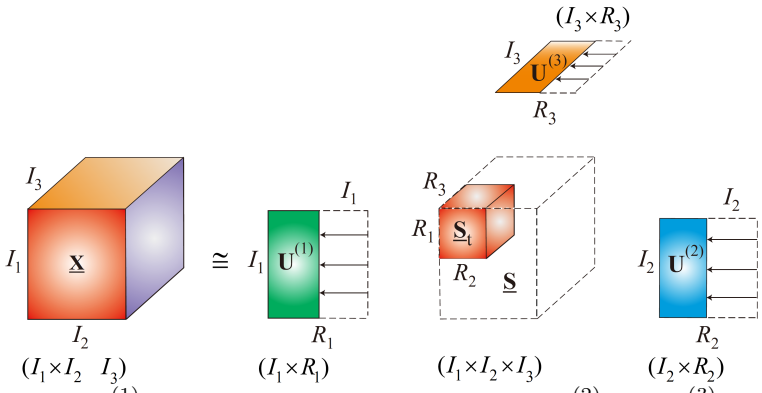
- Components $\mathbf{b}_i^{(1)}, \mathbf{b}_i^{(2)}, \mathbf{b}_i^{(3)}$ (factor 1) are associated with one another (linked)
- But none of them are associated with any other set of such components (factors) for $i \neq j$, e.g. with $\mathbf{b}_R^{(1)}, \mathbf{b}_R^{(2)}, \mathbf{b}_R^{(3)}$.
- Every 'basis' vector has an associated physical meaning, in its respective dimension
- Vectors $\mathbf{b}_1^{(1)}, \mathbf{b}_2^{(1)}, \ldots, \mathbf{b}_R^{(1)}$ can be combined into a factor matrix $\mathbf{B}^{(1)}$ etc., to give

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \lambda_r \cdot \mathbf{b}_r^{(1)} \circ \mathbf{b}_r^{(2)} \circ \mathbf{b}_r^{(3)} = [\![\underline{\mathbf{D}}; \mathbf{B}^{(1)}, \mathbf{B}^{(2)}, \mathbf{B}^{(3)}]\!] \tag{7}$$

Tucker Decomposition (TKD)

TKD with imposed orthogonality constrains ↬ Higher-Order SVD (HOSVD)

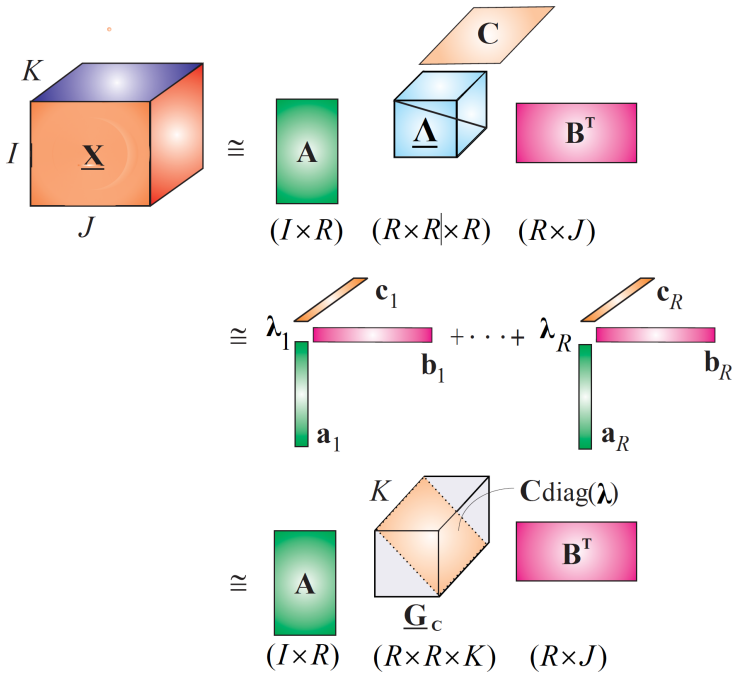
The TKD is not unique, but the subspaces defined by $\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)}$ are unique



- Eeach vector of $\mathbf{U}^{(1)}$ is associated with every vector of $\mathbf{U}^{(2)}$ and $\mathbf{U}^{(3)}$ through the **core tensor** $\underline{\mathbf{S}}$ ↬ $\underline{\mathbf{X}} \approx \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \sum_{r_3=1}^{R_3} \underline{\mathbf{S}}_{r_1 r_2 r_3} \cdot \mathbf{u}_{r_1}^{(3)} \circ \mathbf{u}_{r_2}^{(2)} \circ \mathbf{u}_{r_3}^{(3)}$
- By imposing orthogonality constrains on each factor matrix, we arrive at the natural generalisation of the matrix SVD, the higher-order SVD (HOSVD)
- Low-rank approximation (truncation) is then implemented in analogy with SVD, but separately for each mode, as shown above, where R_1, R_2, R_3 are the truncated ranks

Relation between the CPD and TKD

CPD = TKD with a diagonal core



Beyond standard regression ↬ latent component analysis
The Partial Least Squares (PLS) method

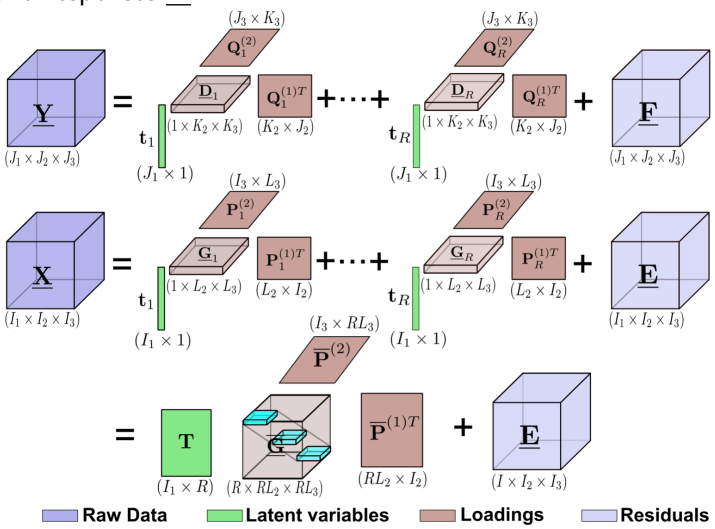
- Regression refers to the modelling of one or more dependent variables (outputs, responses), $\mathbf{Y}$, by a set of independent variables (regressors, predictors), $\mathbf{X}$
- Concept behind PLS ☞ underlying structure is governed by latent variables shared between the $\mathbf{X}$ and $\mathbf{Y}$
- Thus, PLS compromises between fitting $\mathbf{X}$ and predicting $\mathbf{Y}$
- Compare with ARMA(p,q) modelling where the input is white noise (has no structure)

$$\underset{(I\times N)}{\mathbf{X}} = \underset{(I\times R)}{\mathbf{T}}\ \underset{(R\times N)}{\mathbf{P}^{\mathrm{T}}} + \underset{(I\times N)}{\mathbf{E}} = \sum_{r=1}^{R} \boldsymbol{t}_r\, \boldsymbol{p}_r^{\mathrm{T}} + \underset{(I\times N)}{\mathbf{E}}$$

$$\underset{(I\times M)}{\mathbf{Y}} = \underset{(I\times R)}{\mathbf{U}}\ \underset{(R\times M)}{\mathbf{Q}^{\mathrm{T}}} + \underset{(I\times M)}{\mathbf{F}} = \sum_{r=1}^{R} \boldsymbol{u}_r\, \boldsymbol{q}_r^{\mathrm{T}} + \underset{(I\times M)}{\mathbf{F}}$$

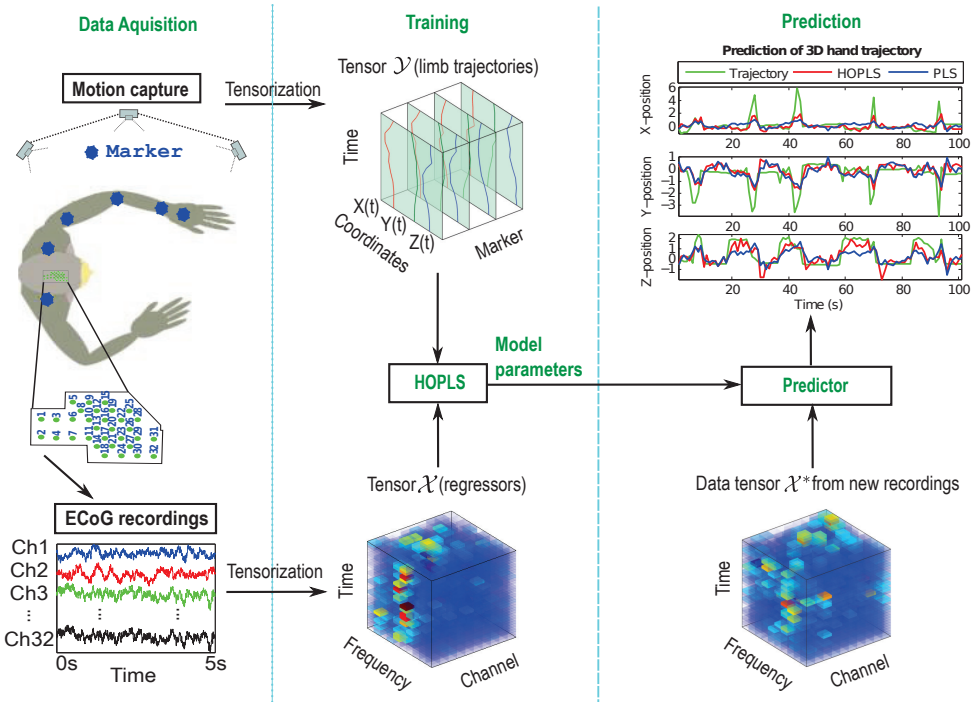
Tensor-valued PLS
The Higher-Order Partial Least Squares (HOPLS)

- Goal: to predict a tensor $\underline{\mathbf{Y}}$ from a tensor $\underline{\mathbf{X}}$
- Approach: to extract the common latent variables between $\underline{\mathbf{Y}}$ and $\underline{\mathbf{X}}$
- Advantages: ability to model interactions between complex latent components of both predictors $\underline{\mathbf{X}}$ and responses $\underline{\mathbf{Y}}$



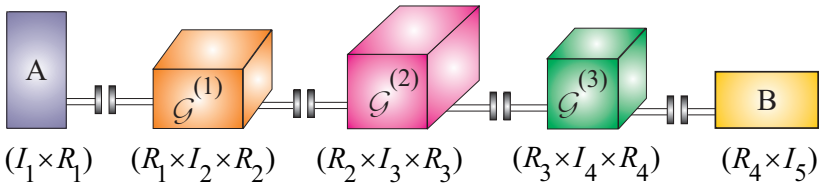
Example 5: Prediction of arm movement from brain activity

Predictors: brain activity. **Responses:** 3-D arm movement trajectory (X,Y,Z)

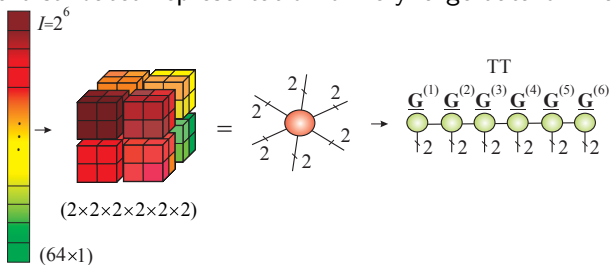


Advanced concepts: Tensor train (TT) decomposition

Curse of dimensionality can be eliminated through tensor network representations

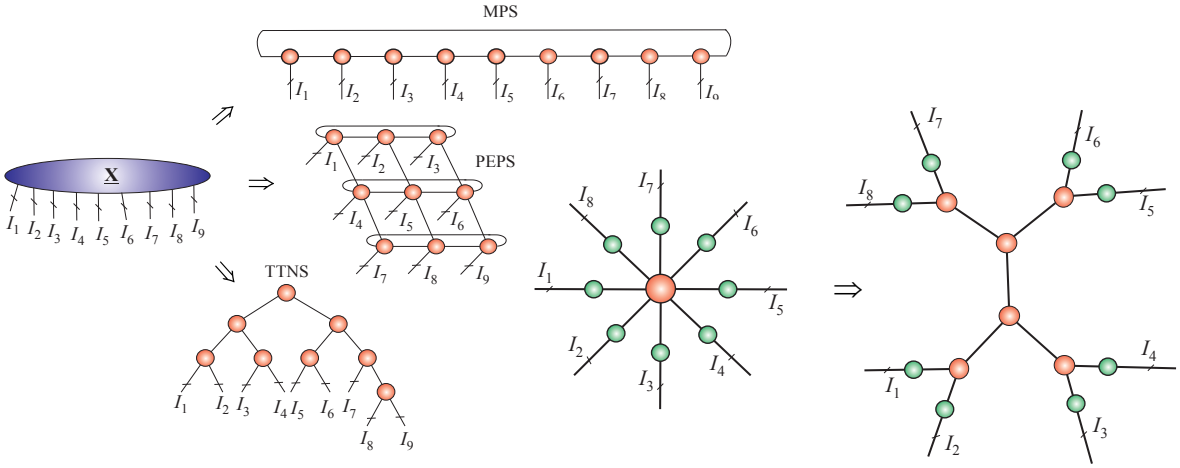


- More degrees of freedom $\rightsquigarrow$ more latent dependencies are preserved
- This inevitably leads to *curse of dimensionality (CoD)* (see Slide 13) $\not\rightsquigarrow$ the number of elements grows exponentially with the the tensor order (number of dimensions)
- TT decomposition represents an Nth-order tensor via two factor matrices, $\mathbf{A}$ and $\mathbf{B}$, and $(N-2)$ small core tensors, $\underline{\mathbf{G}}^i$. These are connected through tensor contractions
- This allows for a distributed representation of very large data on multiple computers



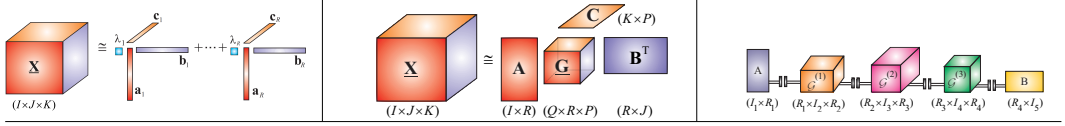
Other types of tensor networks (TNs)

The number of free edges determines the order of a core tensor (usually 3 or 4)



- Tensor network architectures can be with or without loops ↬ the Matrix Product State (MPS), Tree Tensor Network State (TTNS), Projected Entangled-Pair States(PEPS), Hierarchical Tucker (HT)
- TNs decompose a very high-order tensor into sparsely (weakly) connected low-order and small-size core tensors (red circles) ↬ computational and storage benefits

Comparison of multidimensional decompositions



storage complexity

CPD	Tucker	Tensor Train
$\mathcal{O}(NIR)$	$\mathcal{O}(NIR + R^N)$	Depends on a choosen type

inherent structure

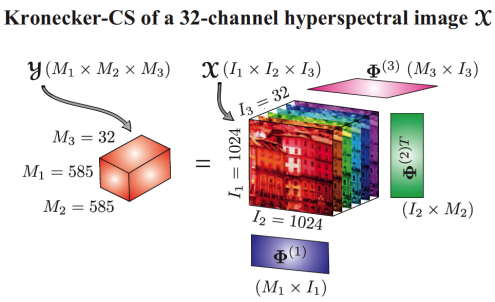
CPD	Tucker	Tensor Train
Represented through rank-1 terms	Represented through core tensors and factor matrices	Represented through tensor contractions

uniqueness conditions

CPD	Tucker	Tensor Train
Very soft and depend on the CPD structure	Constrains should be imposed on factor matrices	N/A

Example 5: Higher-Order Compressed Sensing (HO-CS)

An extension to tensors overcomes the loss of spatial and contextual relationships in data, owing to high degrees of structure inherent in tensors

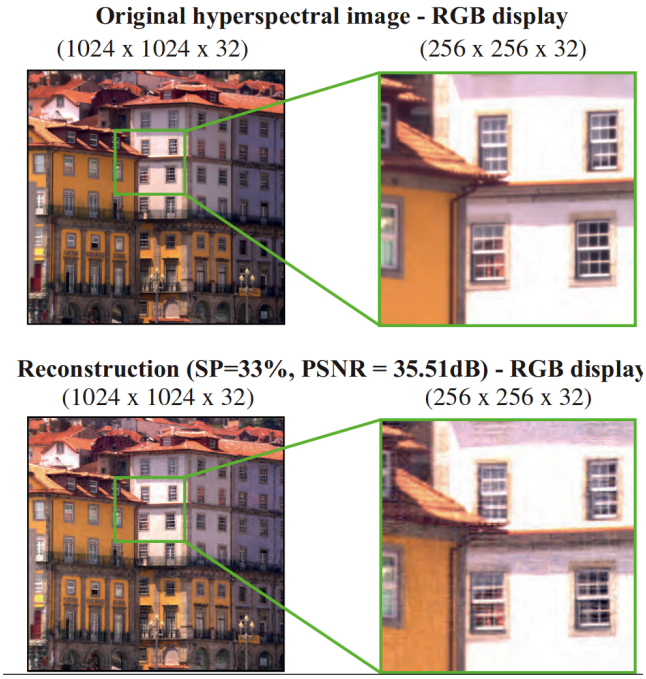


CS $\rightsquigarrow$ signal reconstruction when the set of measurements is much smaller than the original data

Top: Measurement scenario.

Top right: Original huge hyperspectral image.

Bottom: The hyperspectral image of affordable size, reconstructed using HO-CS



Applications across data science

- Civil engineering $\looparrowright$ condition monitoring in structures
- Social networks $\looparrowright$ analysis of information content and information spread
- Multiscale volume visualization $\looparrowright$ integration of tensor decompositions into interactive large-scale volume rendering
- Transportation systems $\looparrowright$ traffic planning and management in intelligent transportation
- Environmental monitoring $\looparrowright$ distributed analysis of ecological parameter spreading at different locations and times
- Internet of things $\looparrowright$ analysis of massive amounts of data captured by embedded devices in large-scale autonomous systems
- Video surveillance $\looparrowright$ crowd density estimation and motion recognition for detection of abnormal activities
- Data fusion $\looparrowright$ combining multiple and diverse data sources to make informed decisions $\looparrowright$ '$1 + 1 > 2$'
- User/topic clustering in text $\looparrowright$ a general tensor model may involve the dimensions e.g. User $\times$ Keyword $\times$ Time
- Network security $\looparrowright$ anomaly via a model Source IP $\times$ Target IP $\times$ Port $\times$ Time

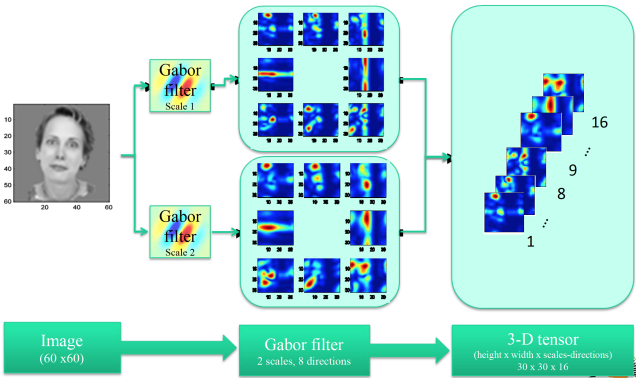
Conclusions

- We have provided an account of multiway analysis of big data
- A particular emphasis has been on tensor decompositions and their applications
- We have elucidate the super-compressions ability of tensor decompositions
- With tensors, the complexity of storage becomes linear, $\mathcal{O}(NIR)$ instead of $\mathcal{O}(I^N)$, where N is the number of dimension in data, R the rank of a tensor, and I the size of the dimensions (modes)
- Application in video analytics
- Application in biomedical processing
- Future perspectives

Literature

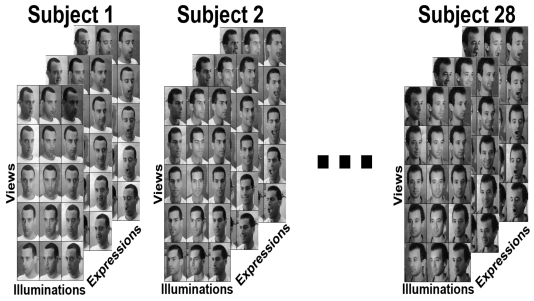
1. T. G. Kolda and B. W. Bader. "Tensor decompositions and applications". SIAM Review, 51(3):455-500, 2009.
2. A. Cichocki, D. P. Mandic, *et al.*, "Tensor decompositions for signal processing applications: From two-way to multiway component analysis", IEEE Signal Processing Magazine, March 2015.
3. Q. Zhao, D. P. Mandic, A. Cichocki *et al.* "Higher order partial least squares (HOPLS): A generalized multilinear regression method". IEEE Transactions on Pattern Analysis and Machine Intelligence, 35(7):1660-1673, 2013a.
4. A. Cichocki, D. P. Mandic, *et al.*, "Tensor networks for dimensionality reduction and large scale optimization. Part 1: Low-rank tensor decomposition", Frontiers and Trends in Machine Learning, 9, (45),249-429, 2016.
5. A. Cichocki, D. P. Mandic, *et al.*, "Tensor networks for dimensionality reduction and large scale optimization. Part 2: Applications and Future Perspectives", Frontiers and Trends in Machine Learning, 2017.

Appendix: Image representation using Gabor filters



- Gabor filter is a linear filter used for edge detection
- The image consists of series of waves of various frequencies
- Each pixel characterizes the intensity of such wave
- The position of a pixel shows the frequency and orientation of the wave
- Extract only waves with a specific frequency and orientation
- Combine them in a 3D array

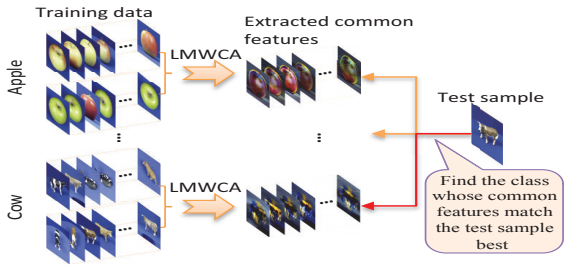
Appendix: Tensor formation through a combination of different characteristics



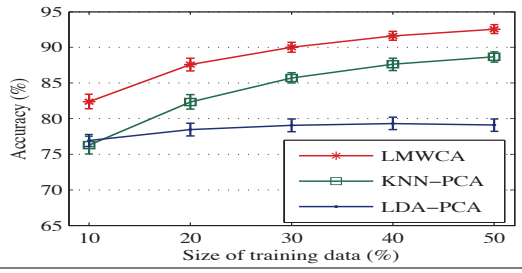
- Face recognition problem is one of the most challenging due to a high variance of parameters such as: view, illumination, expression etc
- At the same time, collected training samples naturally form a multi-dimensional array
- This allows us to extract features that represent dependencies between different modalities

Example 6: Linked Multiway Component Analysis (LMWCA) for classification applications

(a) Sample images from different and same categories



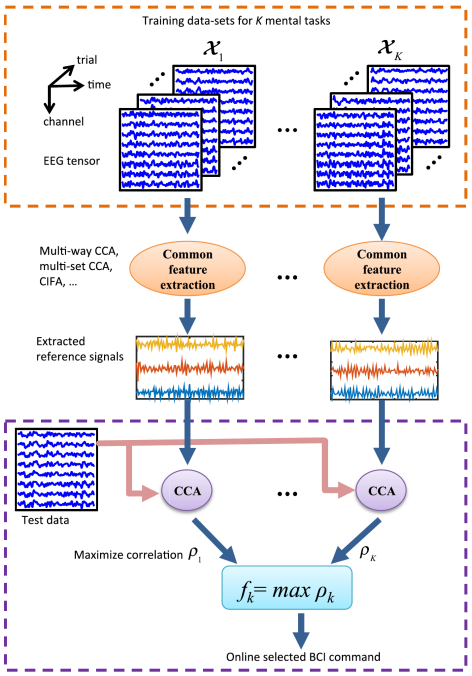
(b) Classification based on LMWCA



(c) Performance comparison

- Data fusion concerns the joint analysis of an ensemble of data sets. For example, human electro-physiological signals in response to a certain stimulus but from different subjects and trials can be grouped together and naturally linked as multi-block data.
- Such data blocks share common information, and at the same time they also allow for individual data features to be kept
- The LMWCA identifies and separates the **common** and **individual** features from the multi-block tensor data and can be a very effective tool for solving classification problems

Example 7: SSVEP recognition in EEG based on Linked Multiway Component Analysis (LMWCA)



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Notes

Notes