Tensor Decompositions and Applications

Blessing of Dimensionality

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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 ↬ 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)
- Tensor networks and their 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^{15} 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 $\looparrowright$ **to make sense from Big Data**?

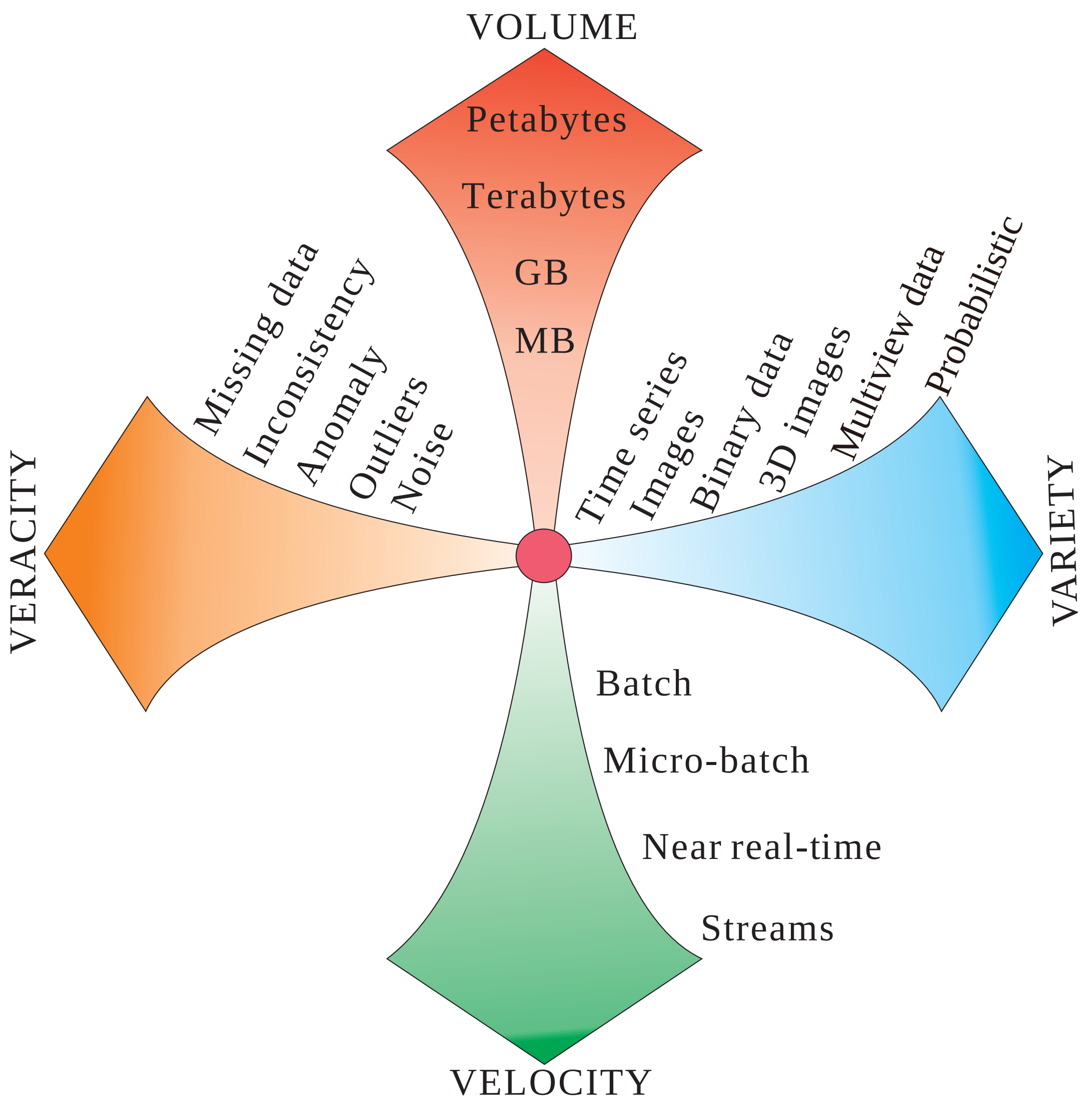
Some facts about Big Data opportunities

According to “Big Data: The next frontier for innovation, competition, and productivity”, published by McKinsey Global Institute in May 2011:

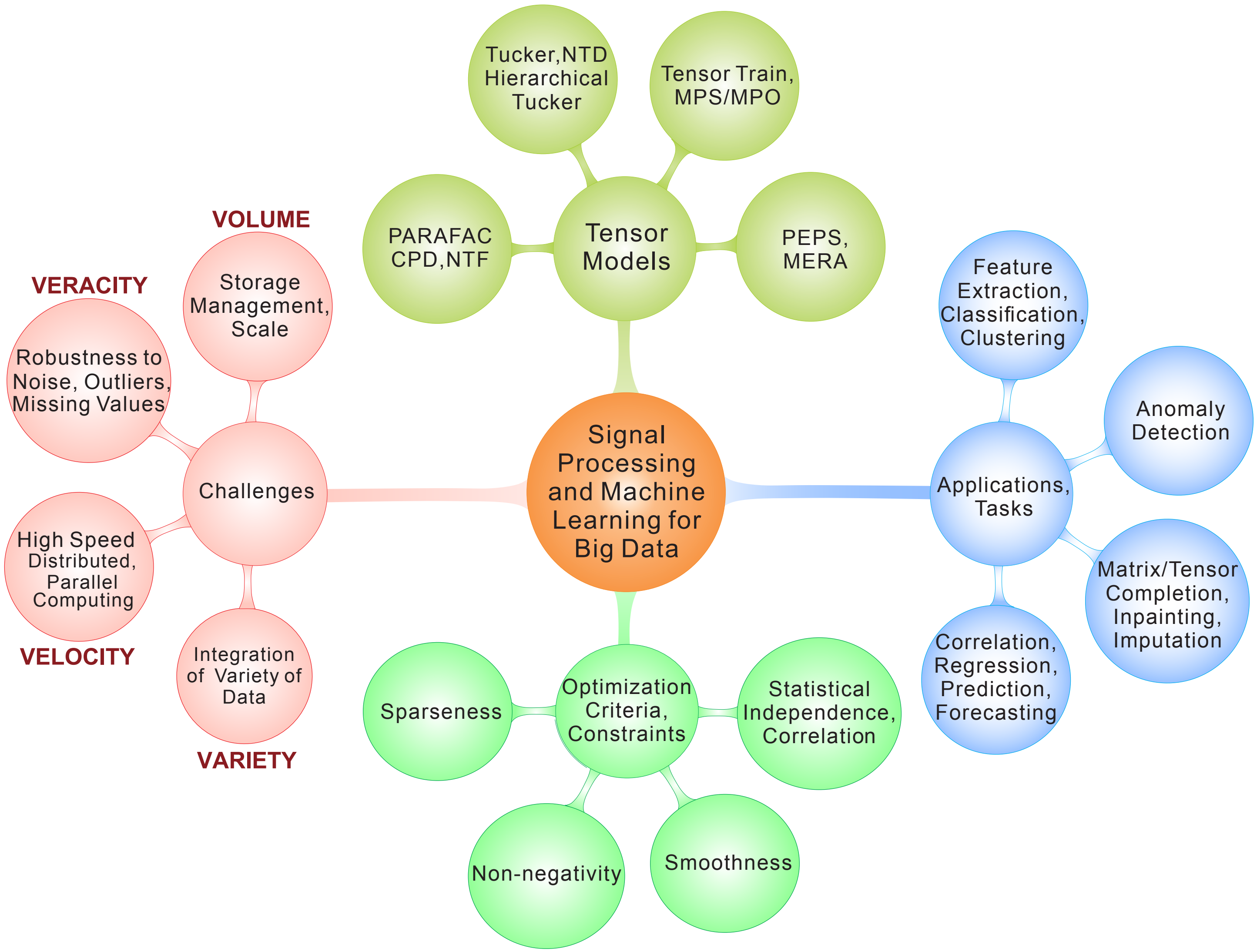
- It would cost USD 600 to by a disk drive which can store all off the music in the world
- In 2010, there were 4 billion mobile phone users in the world
- There is more than 30 billion pieces of content shared on social networks every month
- There is a predicted 40 % growth in global data generated 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), ...



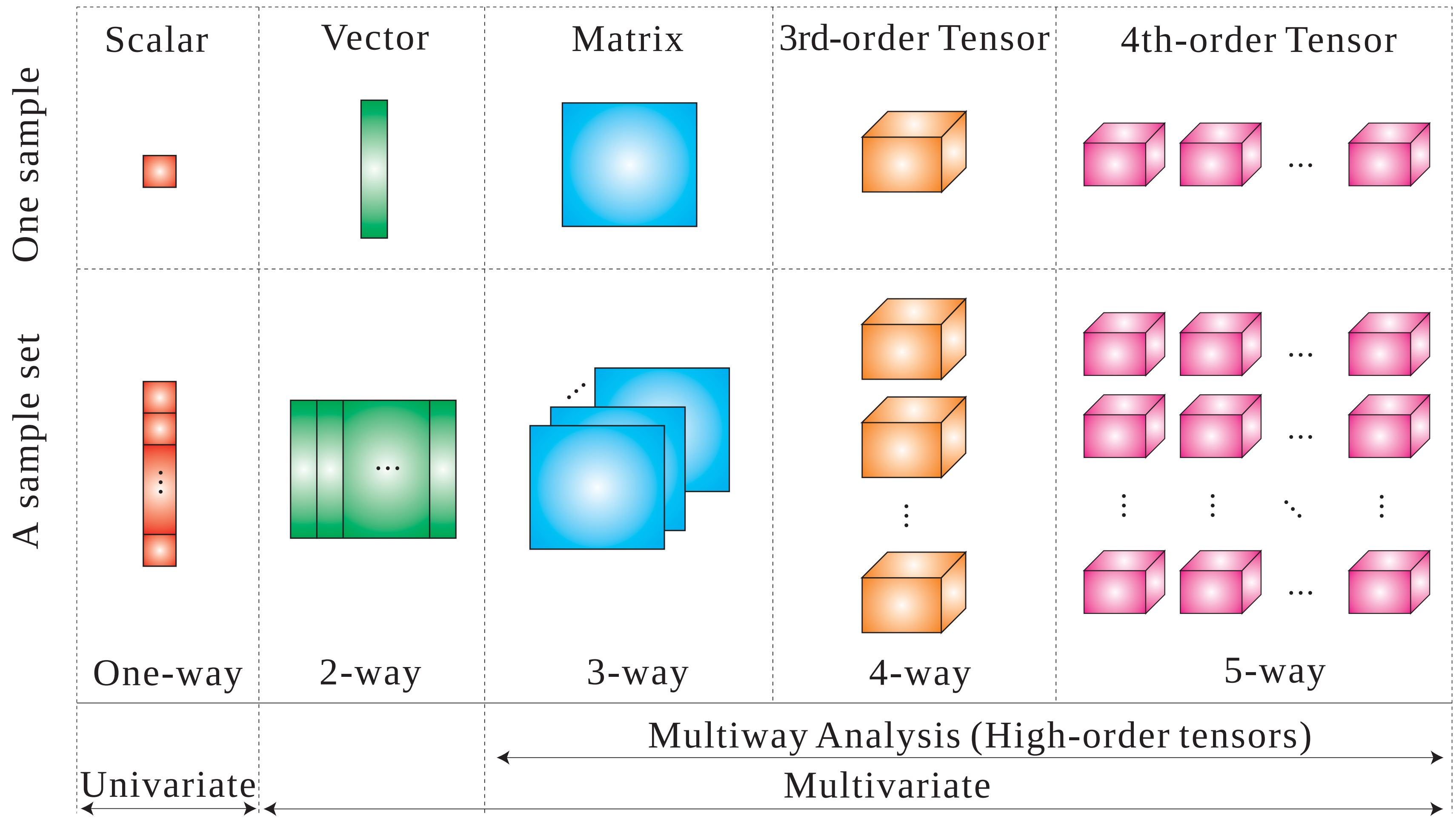
Signal processing an machine learning for big data
Challenges and opportunities



A brief history of Tensors

- The term "tensor" comes from the Latin word *tendere*: to stretch
- Tensors are geometric objects used in Engineering, Mathematics, and Physics as an extension of scalars, vectors, and matrices
- The notion of tensors was first used in the 19th century by William Hamilton to describe concepts of quaternion algebra
- Tensor calculus was introduced in 1900 by Italian mathematician Gregorio Ricci-Curbastro and his PhD student Tullio Levi-Civita
- In 1915, Albert Einstein used tensors in his theory of general relativity for explaining the structure of space-time
- These were later extended by pioneers such as Raymond Cattell and Ledyard Tucker from the 1940s to the 1970s
- American mathematician Frank Hitchcock introduced Tensor Decompositions in 1927
- Other pioneers, Raymond Cattell and Ledyard Tucker, 1940s – 1970s

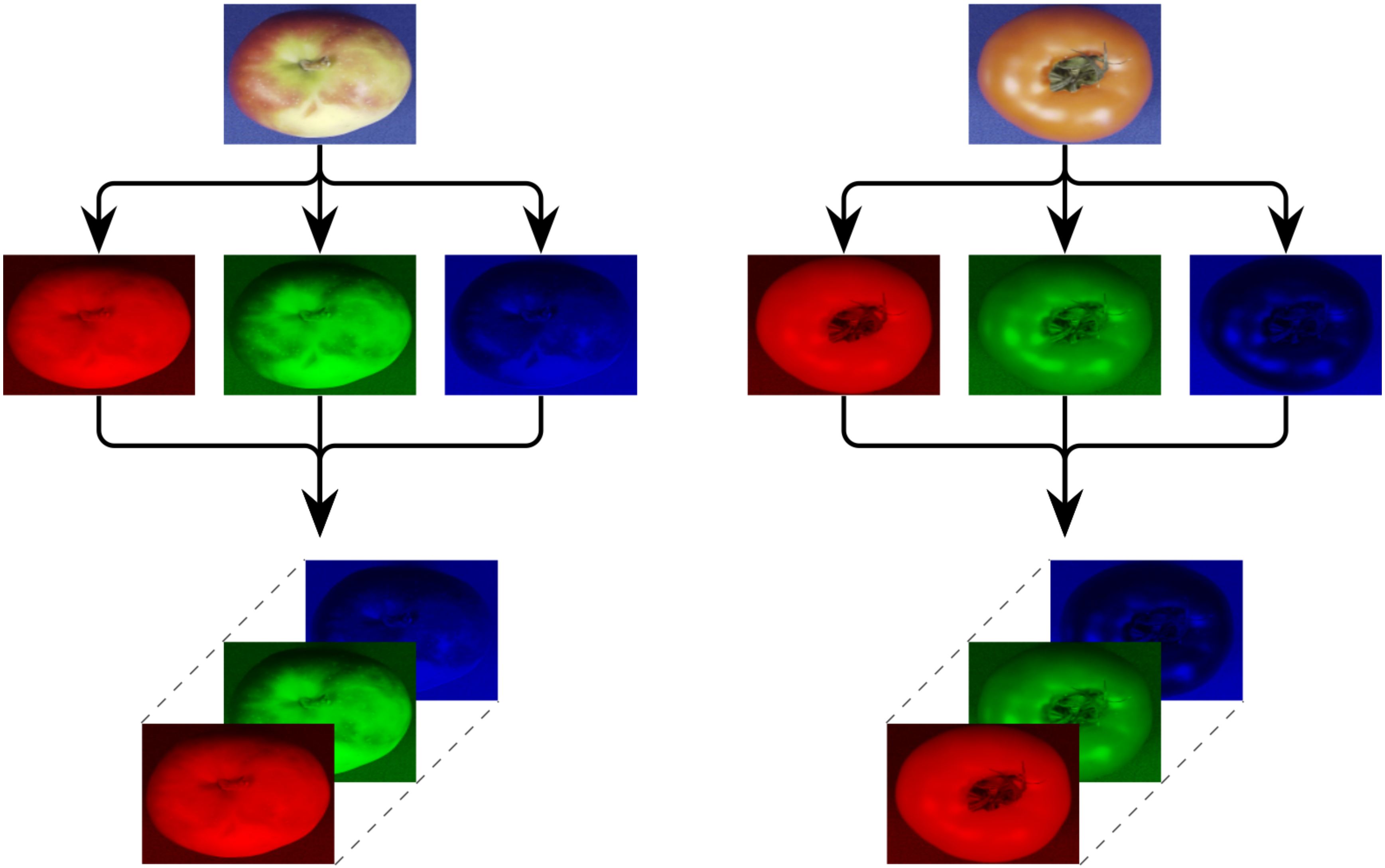
Types of data: From a scalar to a tensor



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

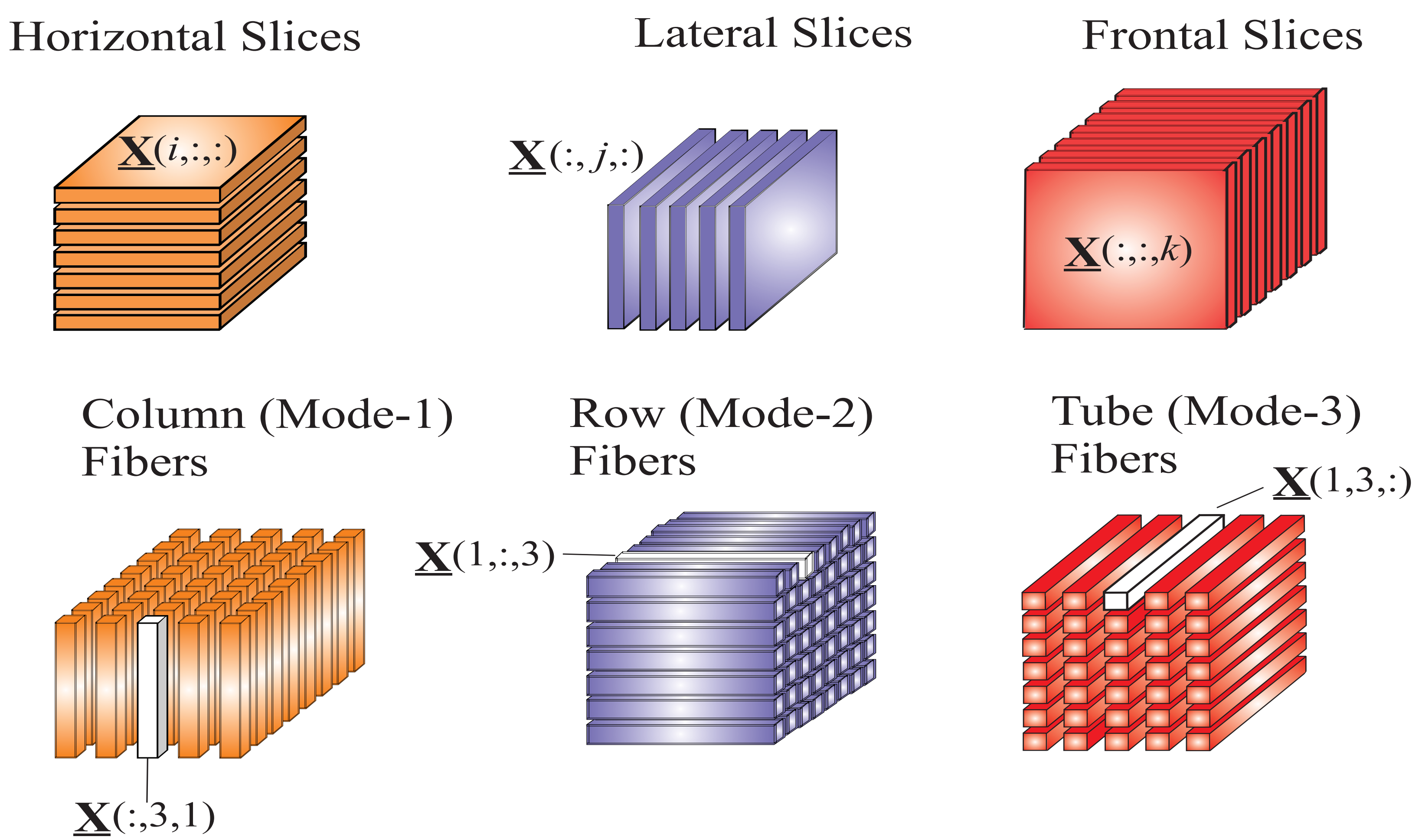
Tensor construction from images

↬ pixel$_X$ × pixel$_Y$ × base color



Sub-structures within tensors

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

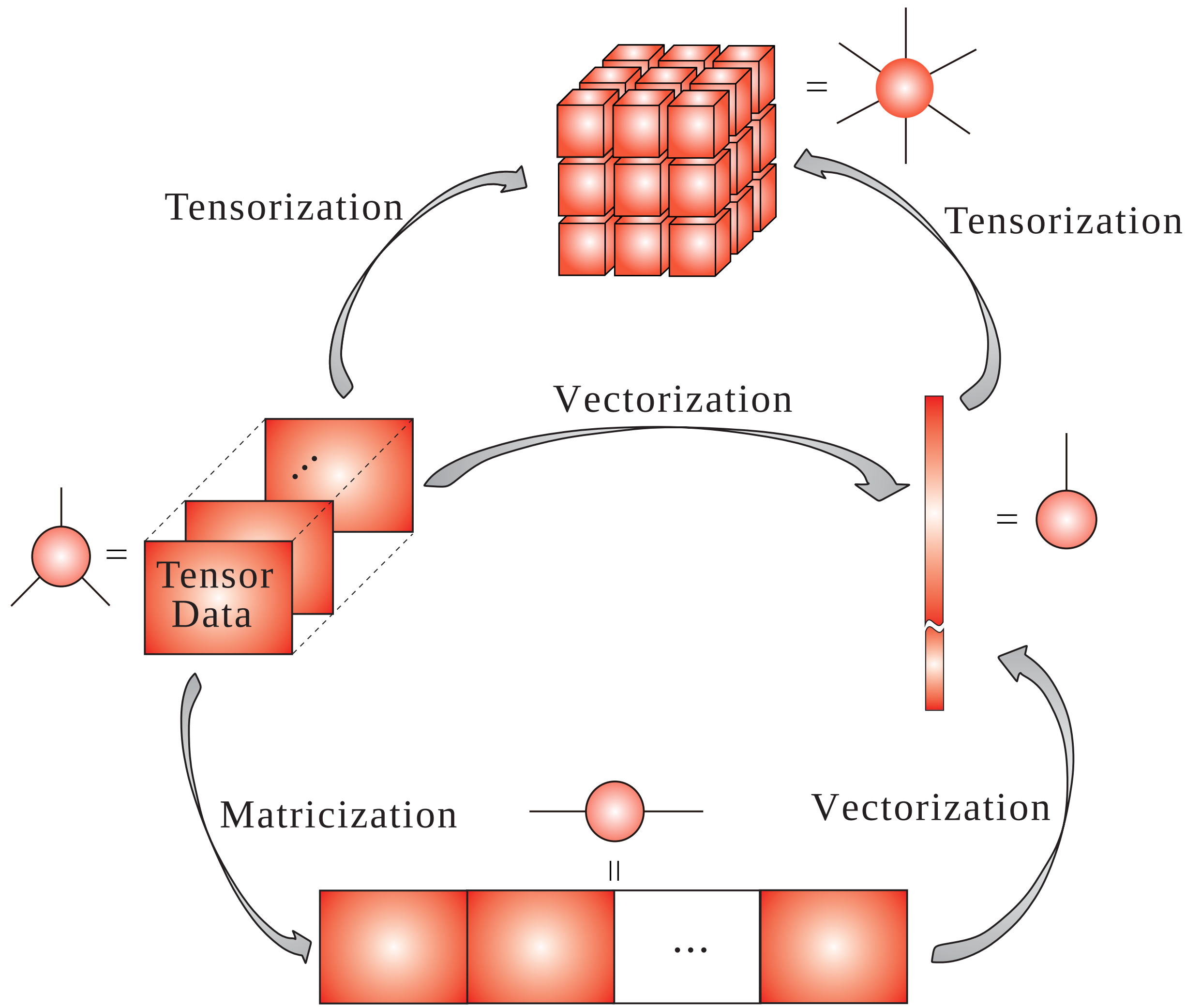


☞ a fiber is produced by fixing two indices and varying one, e.g. $\underline{\mathbf{X}}(1,3,:)$

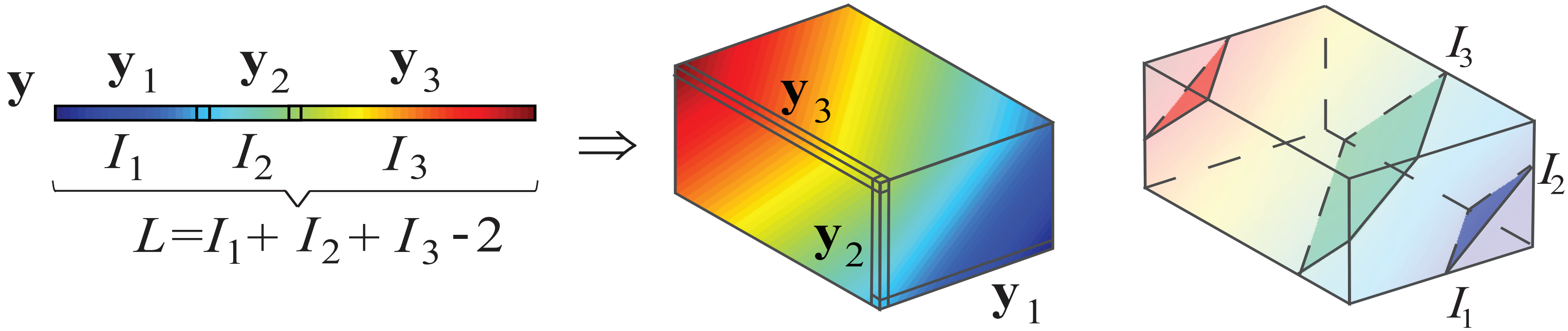
Reshaping of data structures: General concept

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

- One of the advantages of tensors is the flexibility they offer in manipulating data.
- Depending on the application, a tensor can be converted (reshaped) into a matrix, a vector, or another tensor of a different order.
- This is very useful and allows us to apply matrix linear algebra in addition to multi-linear algebra for tensors.



Deterministic folding techniques for structured data ↬ Hankel folding operator



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

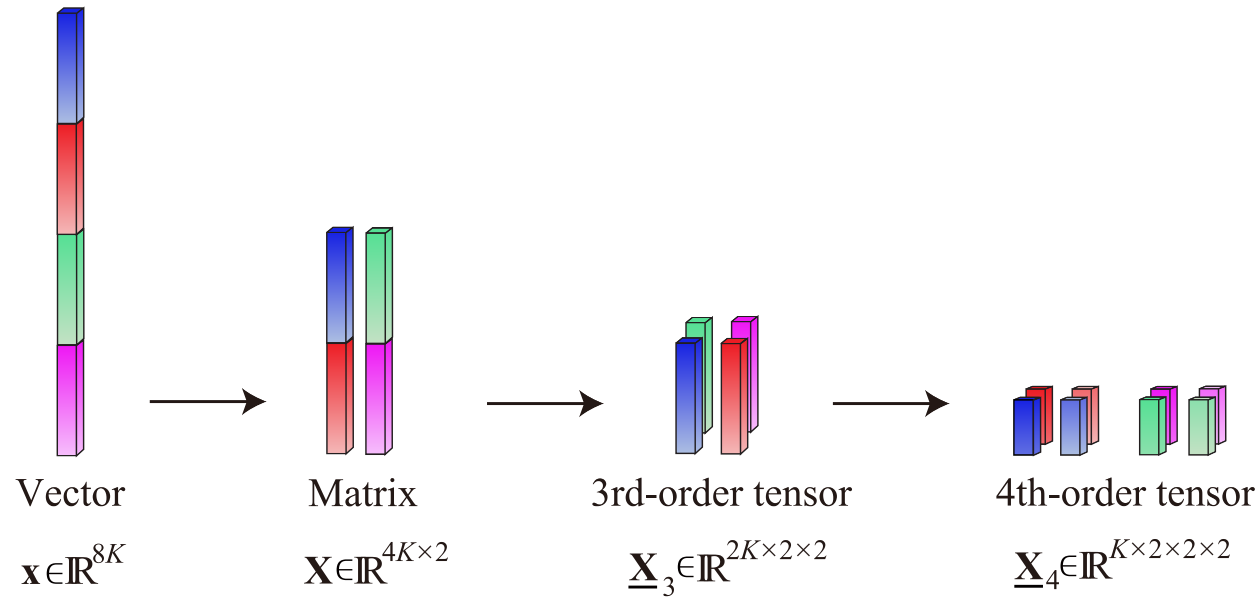
$$\begin{bmatrix} a & az & az^2 & az^3 & \cdots \end{bmatrix} \tag{1}$$

- 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 $\underline{\mathbf{H}}$

Towards tensor networks: 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 56)
- **Mathematical construction**. Through e.g. time x frequency x channel representation
- **Experimental design.** EEG data over I channels, J subjects, K trials (Slides 15-16)
- **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 44)

Example 1: 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 seen as a short & wide matrix $\mathbf{X} \in \mathbb{R}^{1,000 \times 1,000,000}$

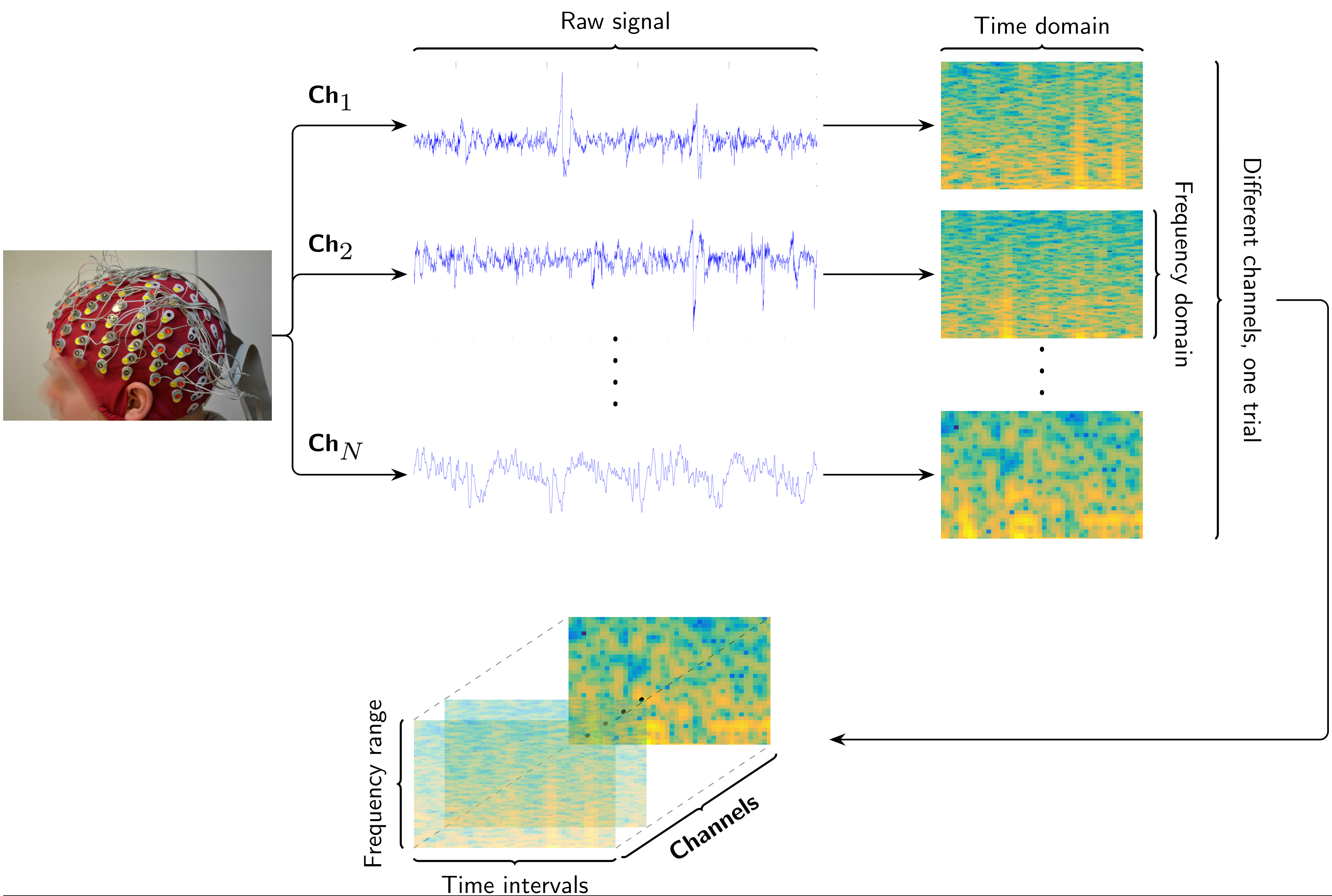
Analysis of all frames at once in this way is not informative or compact

- Significant difference in dimensions ↬ processing is computationally expensive, difficult and not physically intuitive
- Any PCA-type solution would require a matrix of size $10^6 \times 10^6$
- This is a perfect scenario for low-rank tensor approximations and the inherent super-compression capability of tensor representations

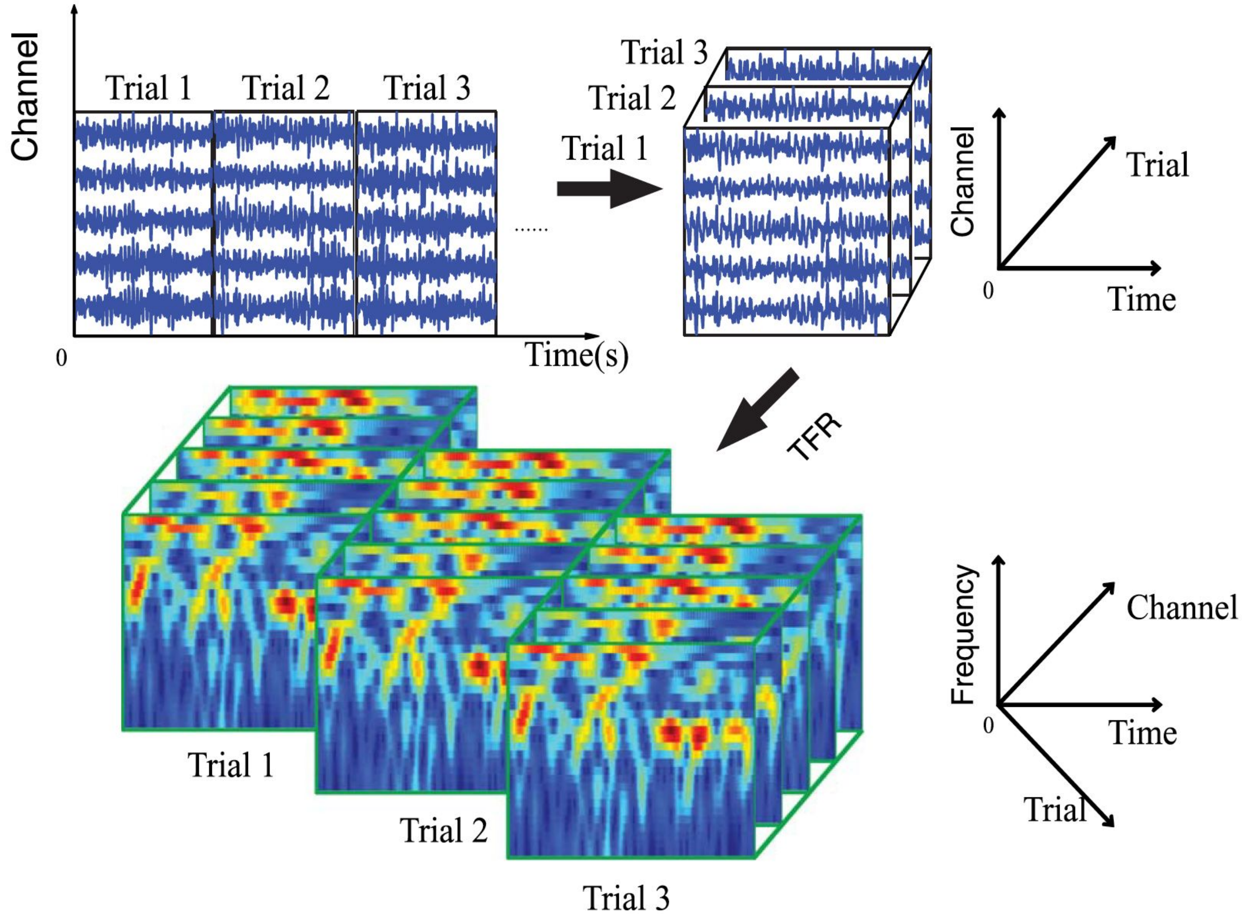
☞ Reshape this awkward-to-analyse data into a compact 3D array

Example 1a: Tensor construction from different channels

↬ channel × frequency × time



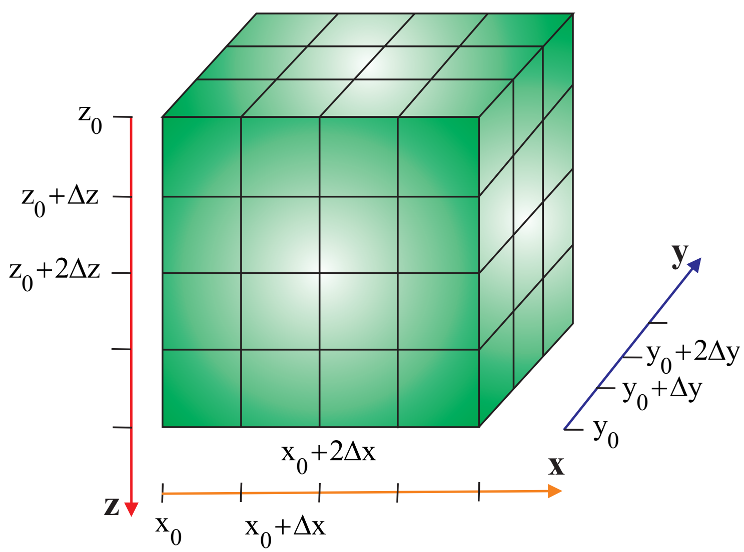
Example 1d: Putting it all together, construction of a 4D tensor with modes channel × trial × frequency × time



- 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

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 2: Scientific computing

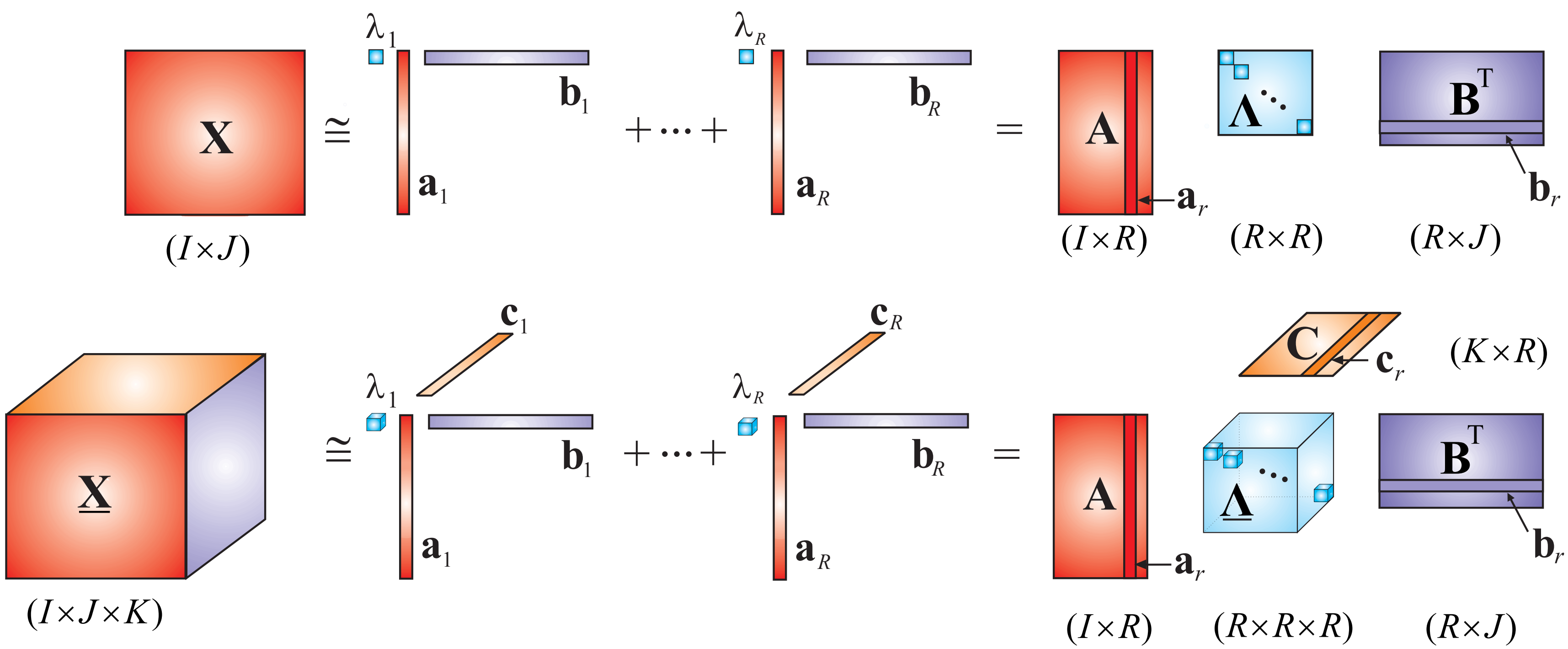
For computational purposes we often need to sample a multidimensional function on a grid (e.g. brain scans)

- 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

Remedy: Canonical Polyadic Decomposition (CPD)

Top: Singular Value Decomposition (SVD) for matrices

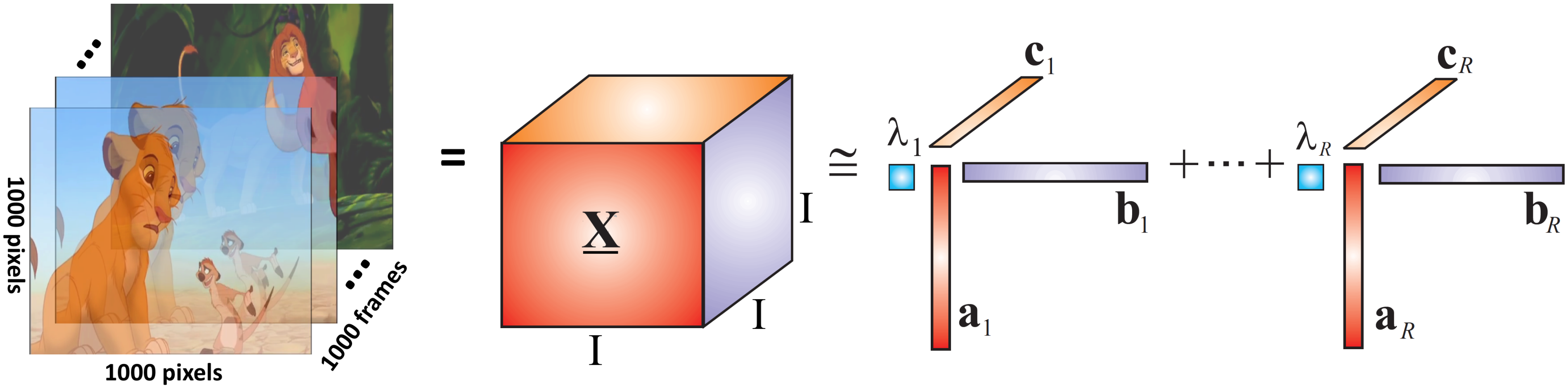
Bottom: Canonical Polyadic Decomposition (CPD) for tensors ↬ tensor rank = R



- 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 3: CPD applied to our video-clip example

Inherent compression within the CPD $\looparrowright$ storage and computational advantages



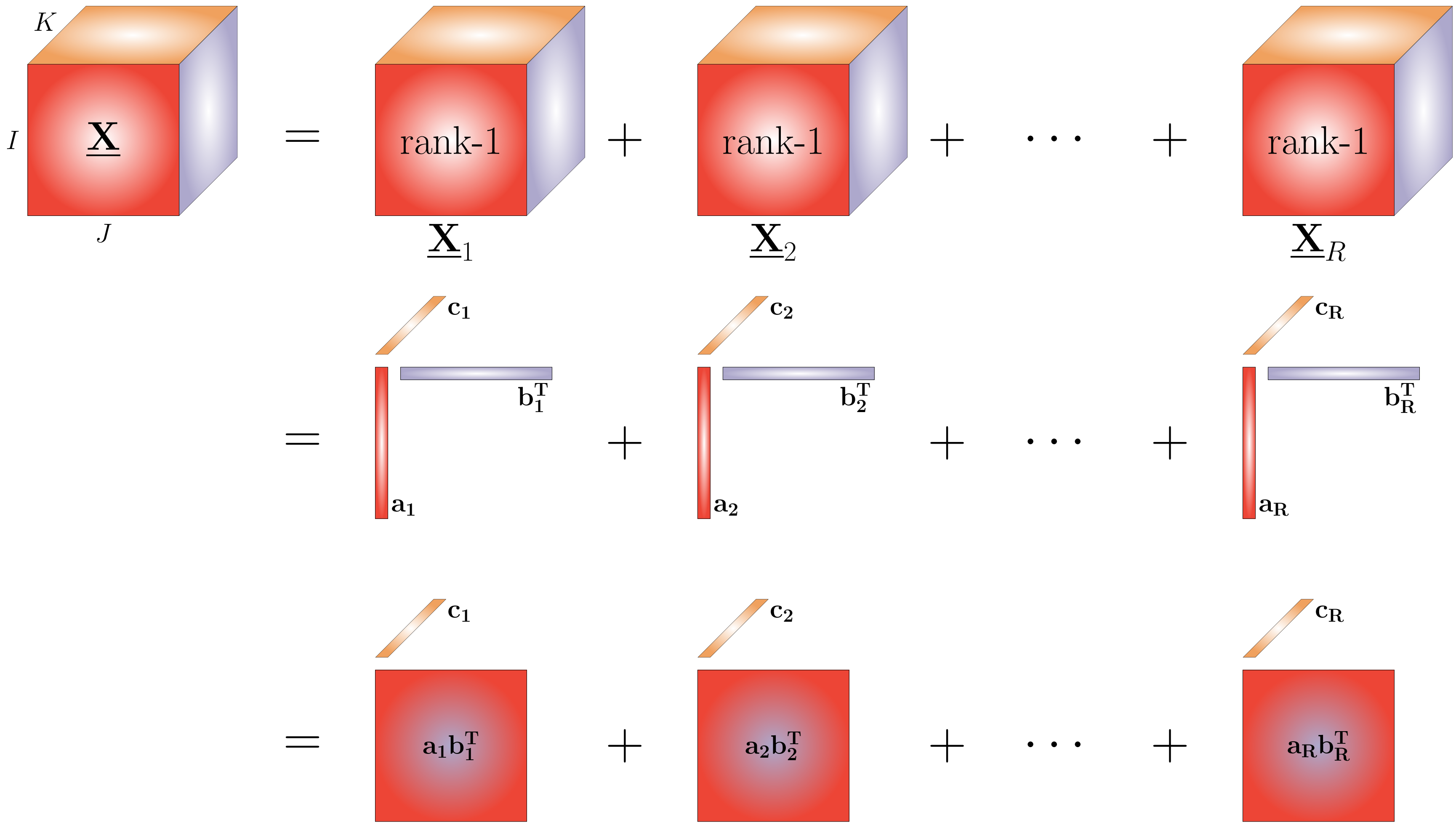
After tensorizing the video clip, tensor order $N = 3$, the dimension in every mode $I = 1000$, and the tensor rank is R. Typically $R \lll I$.

with length($\mathbf{a}_i$)=1000, length($\mathbf{b}_i$)=1000, length($\mathbf{c}_i$)=1000, $\quad i = 1, 2, \ldots, R$

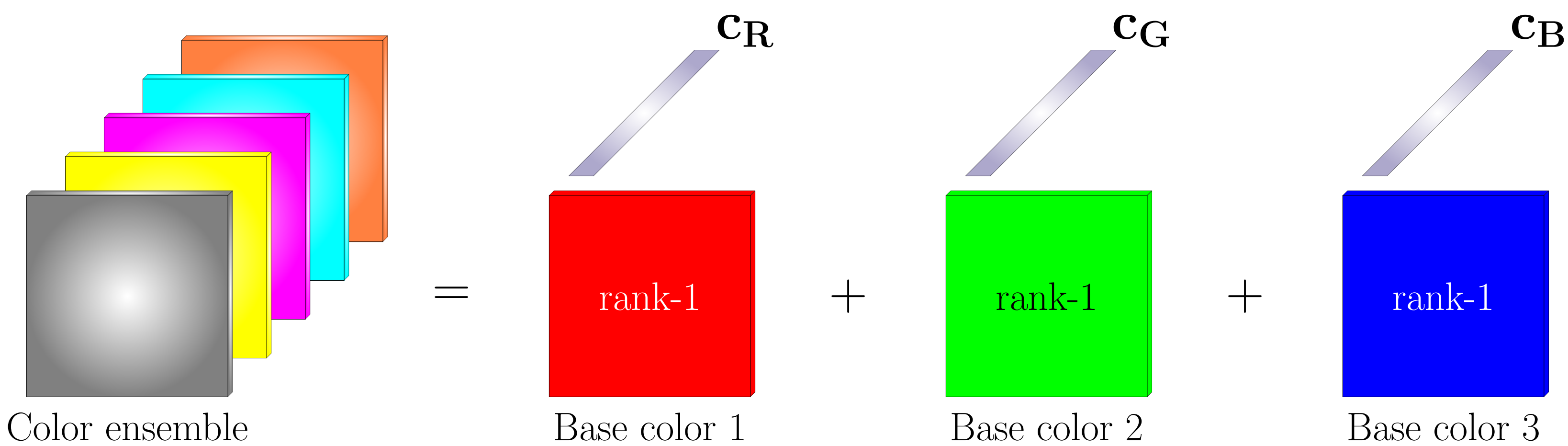
- **Raw data format** $\looparrowright$ $I^N = 1000 \times 1000 \times 1000 = 10^9$ pixels = 1 Giga-pixel
- **In the CPD format**, this becomes $N \times I \times R = 3 \times 1000 \times 10 = 30,000$ pixels (for R=10), that is, compression of almost 5 orders of magnitude
- In scientific computing, if we sample a cube at $I = 10,000$ points, then $I^N = 10^{12}$ raw samples become $N \times I \times R = 3 \times 10^5$ samples in CPD

  For N=4, I=10^4, R=10, the $I^N = 10^{16}$ raw samples $\rightsquigarrow$ 4×10^5 samples in CPD

From matrix rank to tensor rank



Example 4: Intuition behind the tensor rank



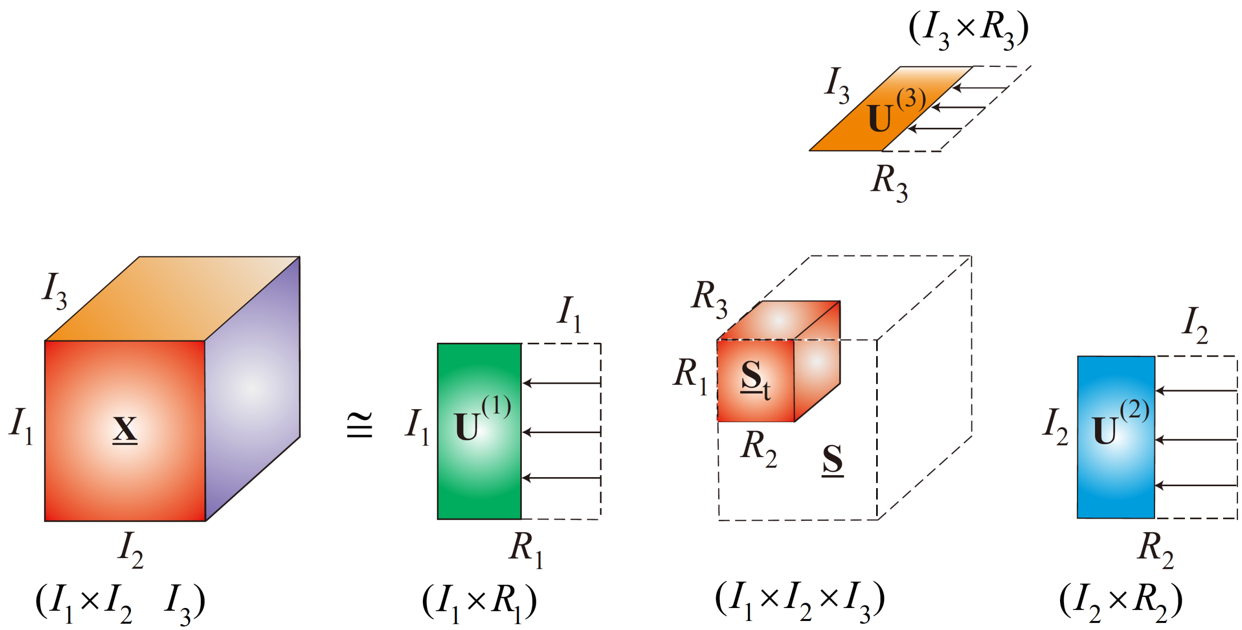
- All colors are just combination of three base colors: red, green and blue $\looparrowright$ rank $= 3$
- Vectors $\mathbf{c}_R, \mathbf{c}_G, \mathbf{c}_B$ represent intensity, i.e. each value characterises how much of the base color there is in the corresponding slice

$$\mathbf{c}_R = \begin{bmatrix} 128 \\ 256 \\ 256 \\ 0 \\ 256 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 1 \\ 1 \\ 0 \\ 1 \end{bmatrix} \qquad \mathbf{c}_G = \begin{bmatrix} 128 \\ 256 \\ 0 \\ 256 \\ 128 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 1 \\ 0 \\ 1 \\ 0.5 \end{bmatrix} \qquad \mathbf{c}_B = \begin{bmatrix} 128 \\ 0 \\ 256 \\ 256 \\ 32 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0 \\ 1 \\ 1 \\ 0.125 \end{bmatrix}$$

Tucker Decomposition (TKD)

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

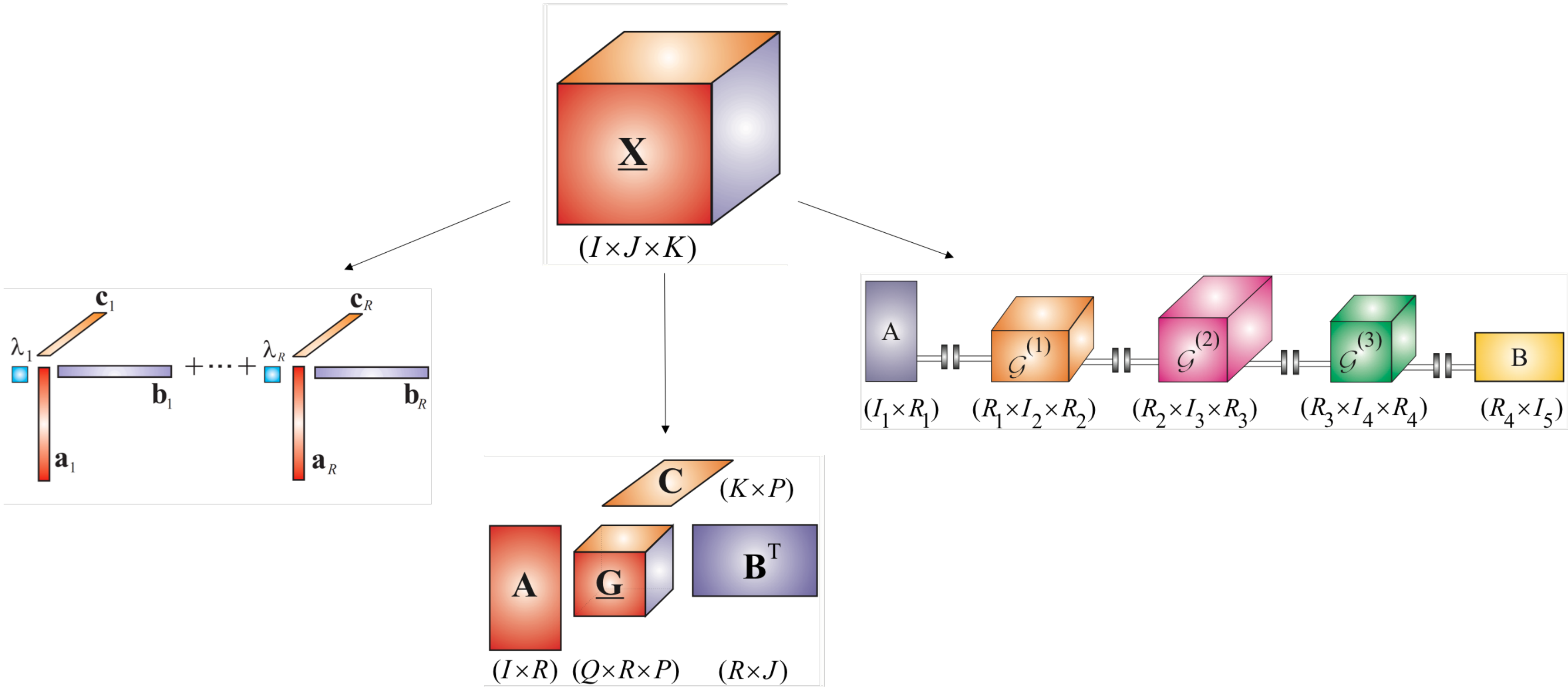
The TKD is not unique, but the subspaces defined by $\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)}$ are unique



- 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

Tensor decompositions ↬ Blessing of dimensionality

From left to right: CPD, Tucker decomposition, Tensor train

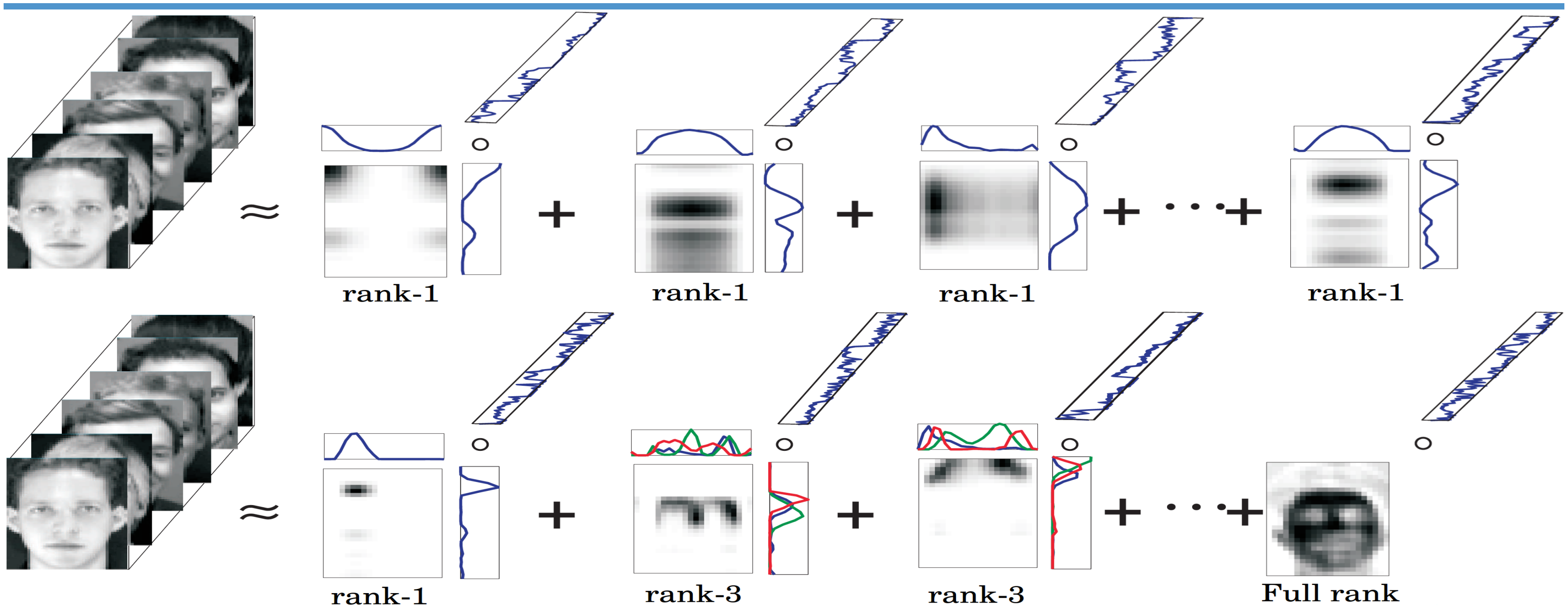


- Can represent tensors with fewer parameters
- Overcome storage issues
- Allow the application of algorithms which would otherwise be prohibitive, to the extremely high computational cost

Block Term Decomposition (BTD)

Combination of the CPD and TKD concepts $\looparrowright$ modeling of complex components

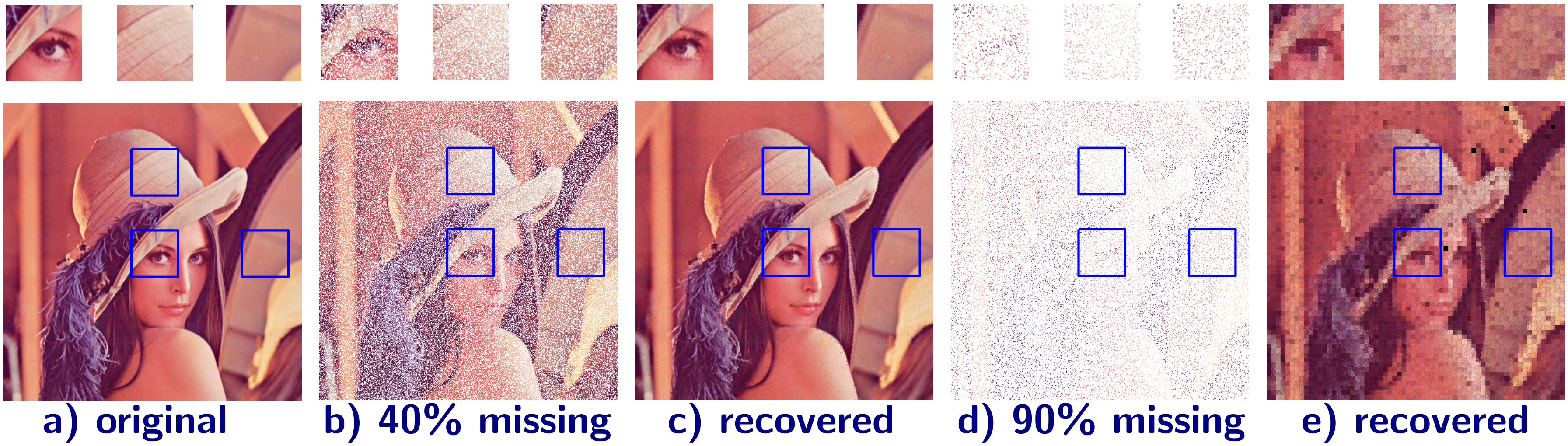
Top: CPD $\rightsquigarrow$ sum of rank-1 tensors **Bottom:** BTD $\rightsquigarrow$ generalization of CPD



- Complexity of basis images varies according to their ranks. **Rank-1** $\looparrowright$ local structures. **Full-rank** $\looparrowright$ more complex structures related to global information
- Combination of basis images with different ranks $\looparrowright$ structures with a range of complexity levels that represent local and global features at the same time
- The BTD is as a sum of tensors with different ranks $\looparrowright$ flexible estimation of data
- Each basic sub-tensor in the sum captures a similar structure (regarding dimensions, sparsity profile and constraints) among all examples in a dataset
- With the same number of features, the BTD approximates data better than the CPD

Example 5: Tensor completion (missing data recovery)

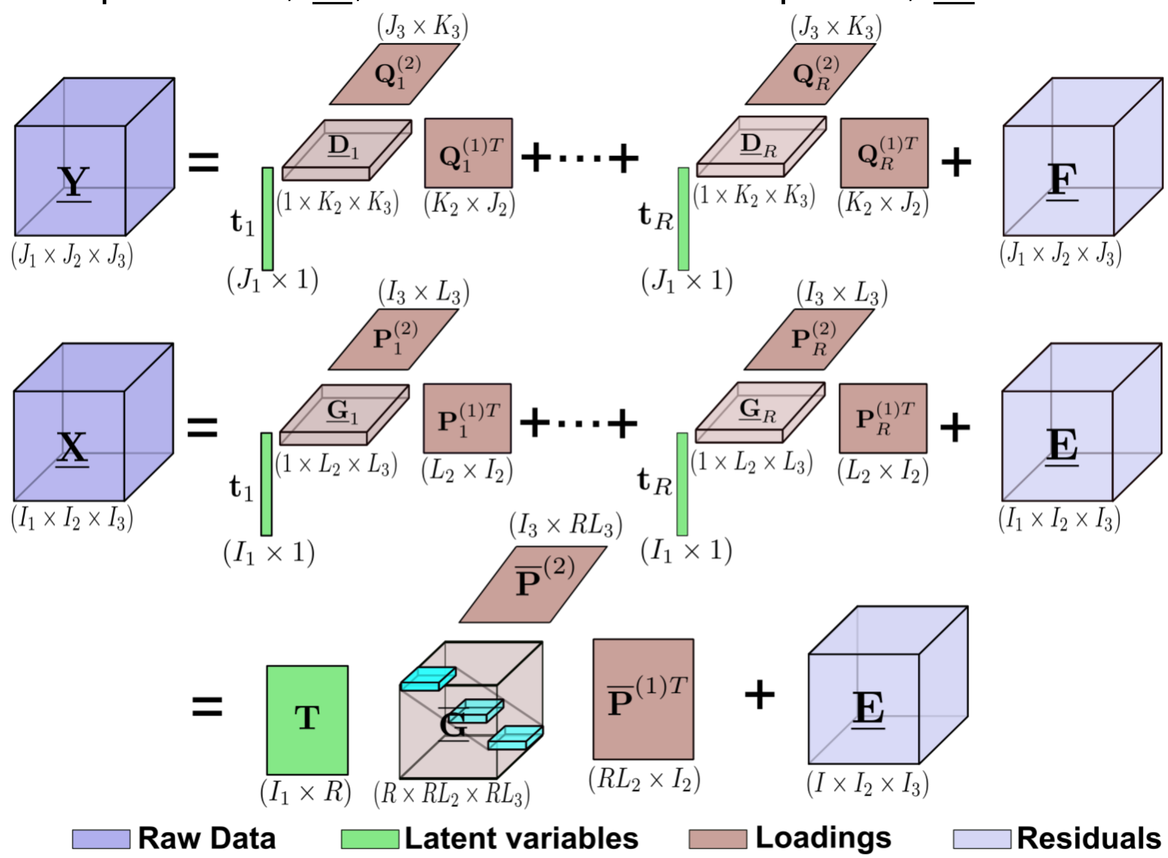
A type of BTD (Kronecker BTD) recovers an image with even 90 % missing data



- Missing data may arise due to faulty or unrealiable sensors (Veracity, see Slide 5)
- Missing data recovery is based on the available information (inpainting)
- The RGB image is a natural tensor (see Slide 13), in this case of size $512 \times 512 \times 3$
- For data with structure, like the above image, TDs can peform missing data recovery whereby the missing pixels are recovered through a Kronecker product of available pixels and an "indicator tensor" (binary mask determined by available/mixing pixels)
- Observe good results with even 90% of missing pixels
- The problem of data reconstruction from incomplete information is closely related to the Compressed Sensing paradigm (see Slide 44)

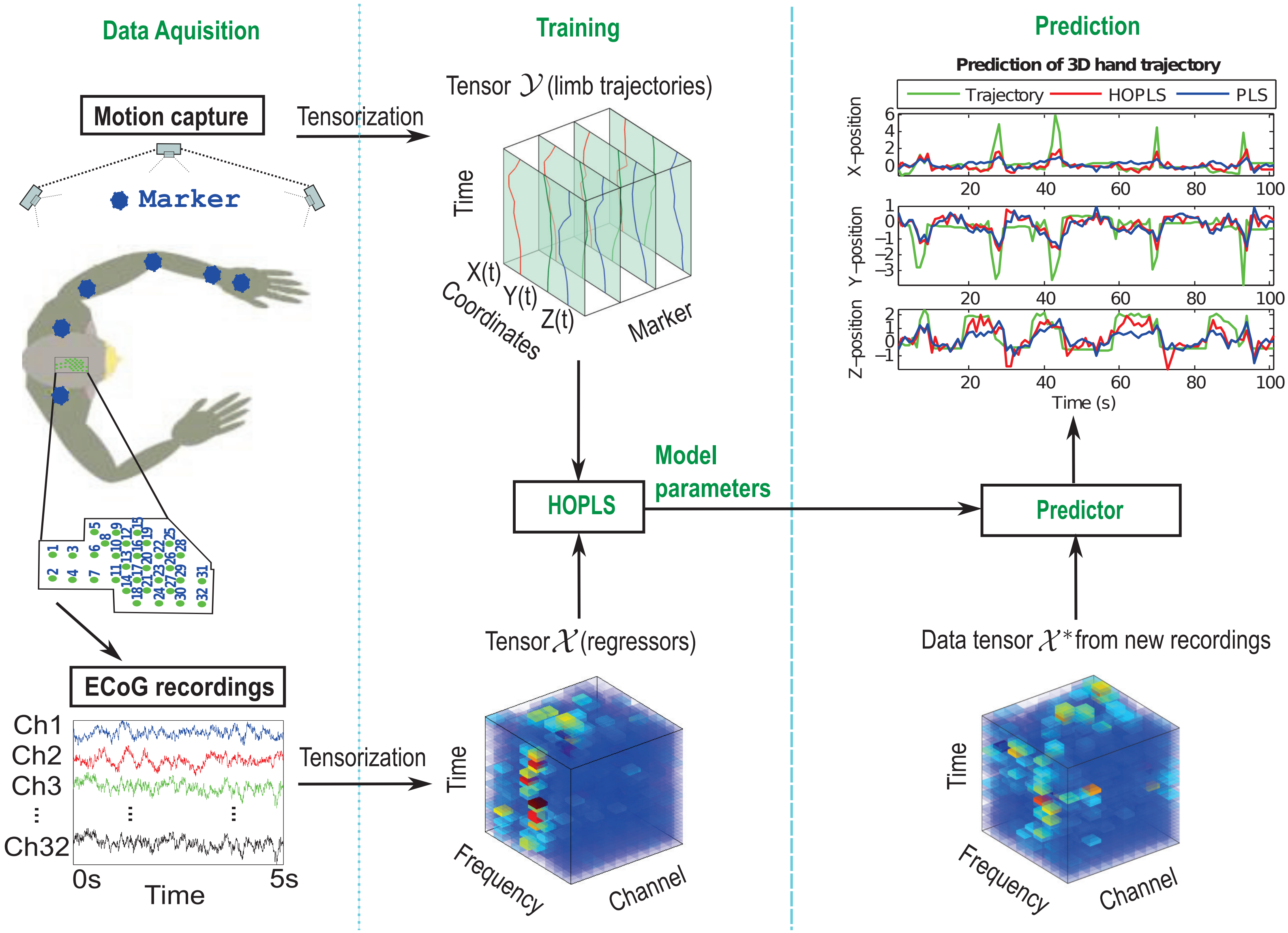
Beyond standard regression ↬ Tensor-valued PLS
The Higher-Order Partial Least Squares (HOPLS)

- **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 the tensor of predictors, $\underline{\mathbf{X}}$, and the tensor of responses, $\underline{\mathbf{Y}}$



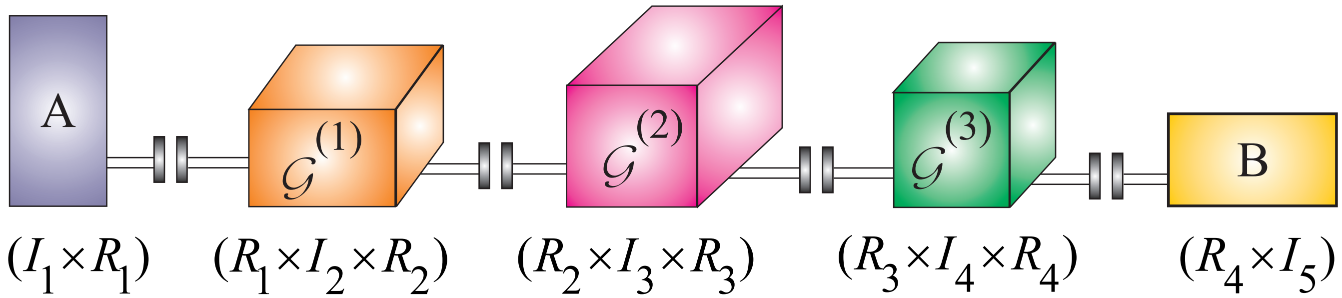
Example 6: Prediction of arm movement from brain activity

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

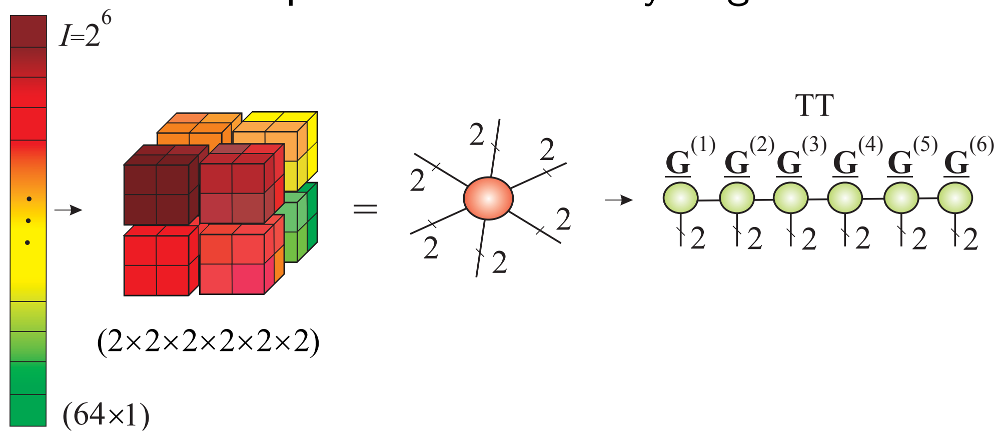


Advanced concepts: Tensor train (TT) decomposition

Curse of dimensionality can be eliminated through tensor network representations

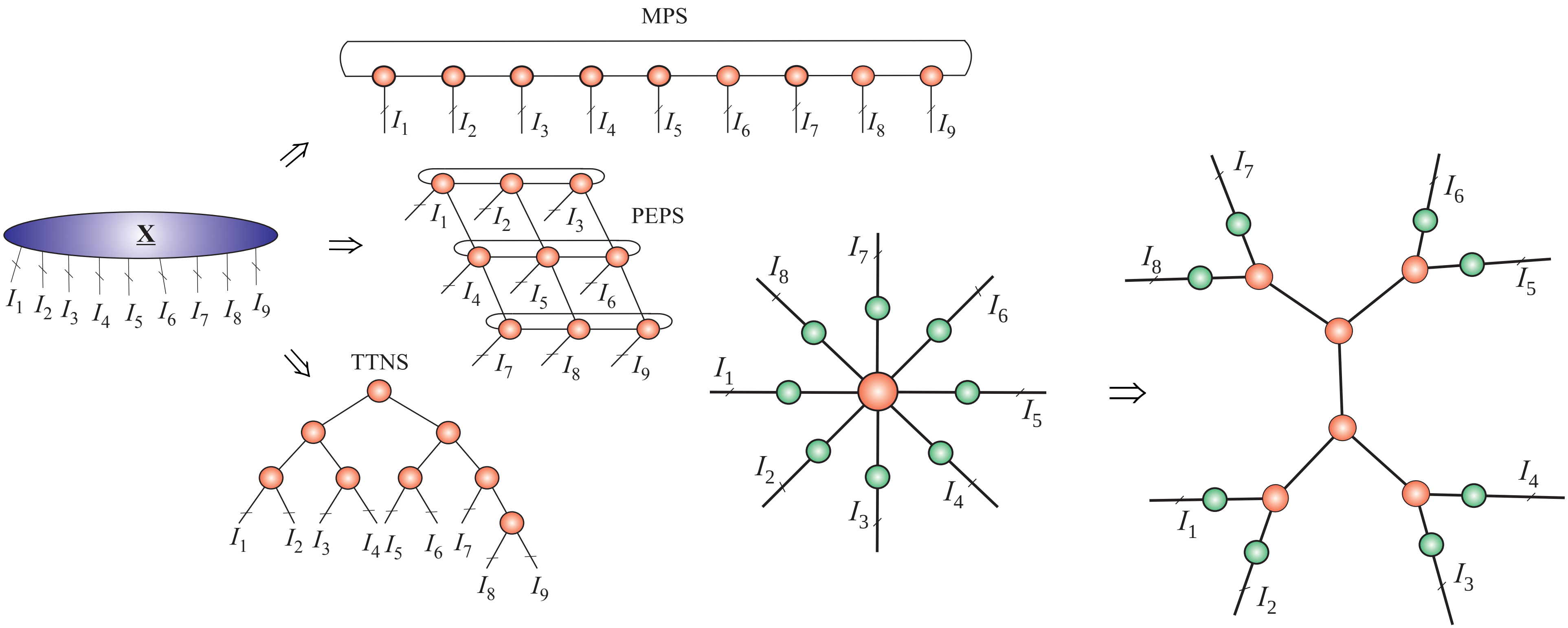


- More degrees of freedom $\rightsquigarrow$ more latent dependencies need to be preserved
- This inevitably leads to *curse of dimensionality (CoD)* (see Slide 17) $\looparrowright$ the number of elements grows exponentially with the the tensor order (number of dimensions)
- TT decomposition represents 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)

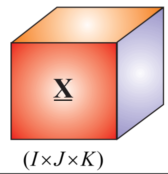
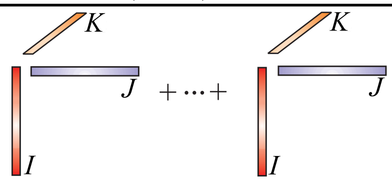
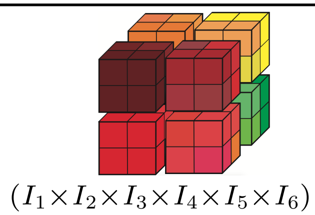
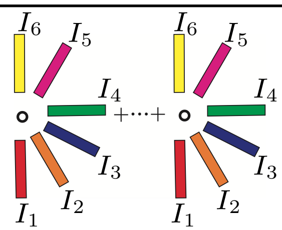
The number of free edges determines the order of a core tensor (usually 3 or 4)



- 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

Super-compression inherent to TNs

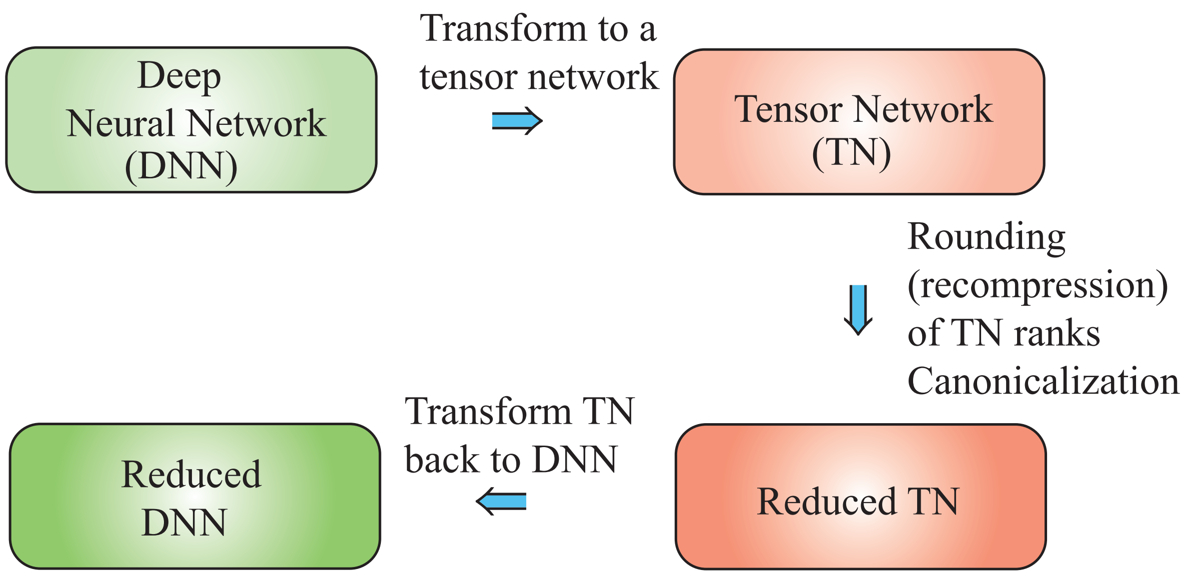
Exponential complexity for the raw data format ⇝ linear complexity for TDs

Data format	length(mode$_n$)=10	length(mode$_n$)=10^m	General case
	10^3	10^{3m}	IJK
	$R \cdot 3 \cdot 10$	$R \cdot 3 \cdot 10^m$	$R(I+J+K)$
	10^6	10^{6m}	$\prod_{n=1}^{6} I_n$
	$R \cdot 6 \cdot 10$	$R \cdot 6 \cdot 10^m$	$R\sum_{n=1}^{6} I_n$

Number of elements in a data format

- R is the rank of a tensor $\underline{\mathbf{X}}$ ↬ CPD is a sum of R rank-1 terms. On practice $R \ll I_n$
- For an N^{th}-order tensor all I^N elements are efficiently represented through the CPD as a linear (instead of exponential) function of number of elements in each mode

Opening the DNN blackbox ↬ From neural networks to tensors and tensor networks



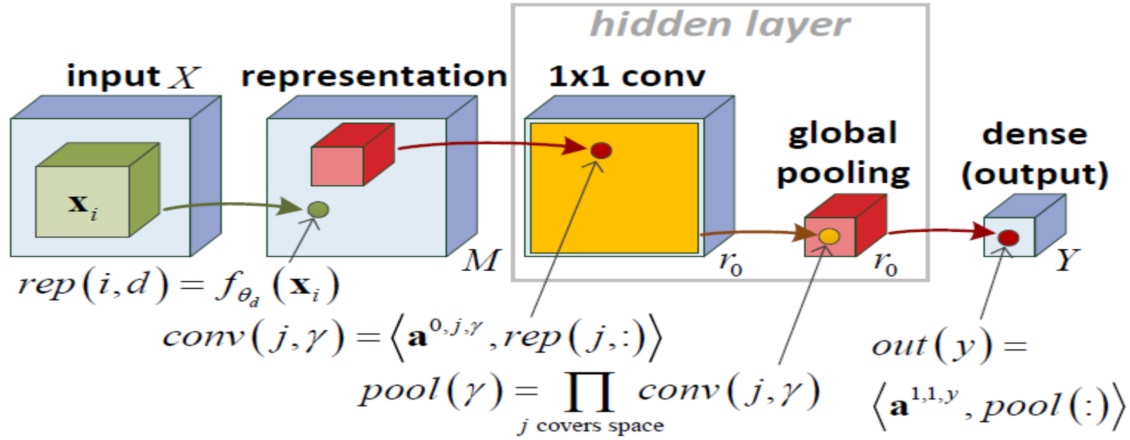
Depth efficiency ↬ DNNs can implement with polynomial size computations that would require super-polynomial size for shallow NNs.

☞ As a consequence, the deeper the network the better the performance

Problem: It is unclear to what extent convolutional neural networks leverage depth efficiency, what is the size of a deep network to perform computations not achievable by shallow networks?

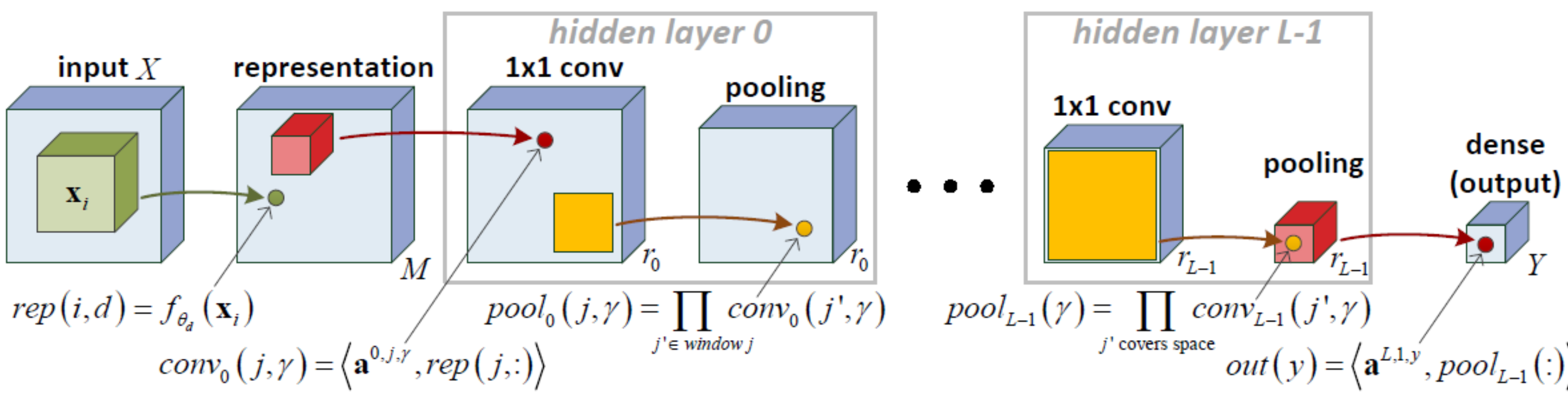
Opening the black box of Neural Networks

Cohen and Shashua: Shallow and deep networks vs. tensors



The weight tensor $\underline{\mathbf{A}}$ of this shallow network is given by the standard CPD

$$\underline{\mathbf{A}} = \sum_{\gamma=1}^{r_0} a_\gamma^{1,1,y} \mathbf{a}^{0,1,\gamma} \circ \mathbf{a}^{0,2,\gamma} \circ \cdots \circ \mathbf{a}^{0,N,\gamma}$$



The weight tensor $\underline{\mathbf{A}}$ of this deep network is a tensor train (HTD)

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

Currently available software for multilinear analysis

- **HOTTBOX**: Higher Order Tensors ToolBOX. Python library for tensor decompositions, statistical analysis, visualisation, feature extraction, regression and non-linear classification of multi-dimensional data.
  (Under active development, contact ik1614@ic.ac.uk, d.mandic@imperial.ac.uk)

- **TensorLab**: the toolbox builds upon the complex optimization framework and offers numerical algorithms for computing the CPD, BTD, and TKD; the toolbox includes a library of constraints (e.g., non-negativity and orthogonality) and the possibility to combine and jointly factorize dense, sparse, and incomplete tensors

- **TensorLy**: is a fast and simple Python library for tensor learning

- **Tensor Train (TT) -Toolbox**: contains several important packages for working with the TT-format. It is able to do TT-interpolation, solve linear systems, eigenproblems, solve dynamical problems.

Conclusions

- Multiway data representation and the associated multilinear algebra are a natural way to approach the Big Data paradigm
- Representation of data through higher-order tensors is both physically meaningful and yields storage and computational advantages
- A particular emphasis has been on tensor decompositions (Canonical Polyadic, Tucker) and their applications
- The associated low-rank tensor approximations enable super-compression in tensor formats, thus aleviating or completely eliminating the **curse of dimensionality** associated with Big Data
- With tensors, the complexity of storage becomes linear, $\mathcal{O}(NIR)$, instead of the exponential, $\mathcal{O}(I^N)$, complexity in the raw data format, where N is the number of dimensions in data, R the rank of a tensor, and I the size of the dimensions (modes)
- Tensor networks $\looparrowright$ distributed storage and computing of otherwise unmanageable volumes of data
- Applications $\rightsquigarrow$ video analytics, biomedical eng., social networks, ...

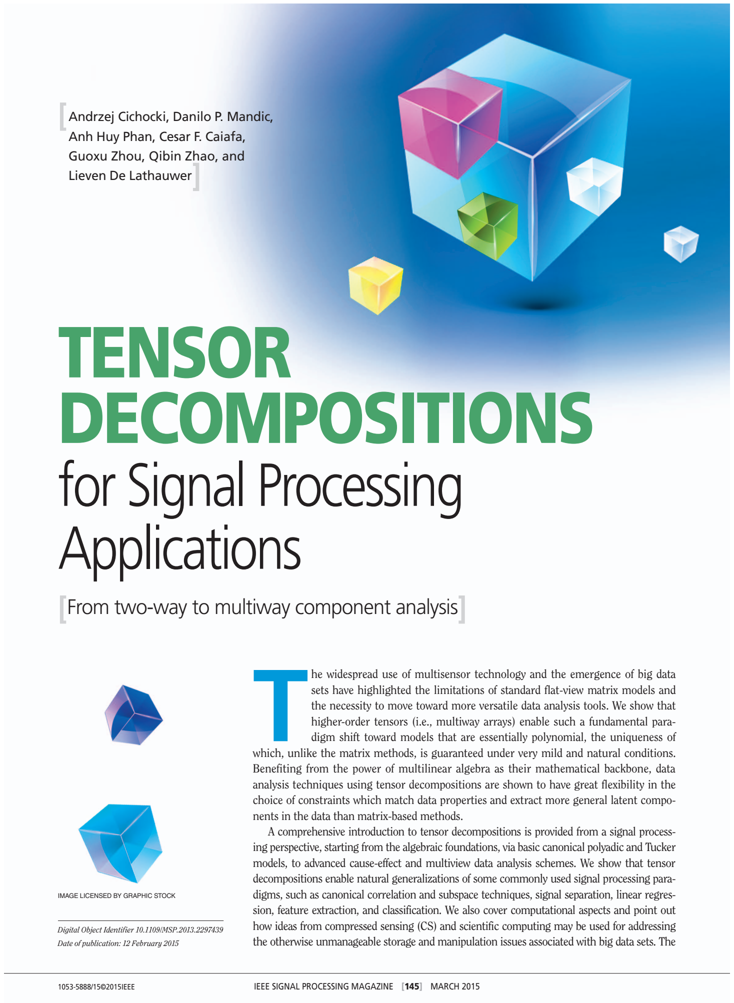
Literature

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, 32(2):145-163, 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, 2013.
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.
6. L. De Lathauwer, *et al.*, "A multilinear singular value decomposition", SIAM Journal on Matrix Analysis and Applications 21(4):1253-1278, 2000.
7. J. B. Kruskal, "Three-way arrays: rank and uniqueness of trilinear decompositions, with application to arithmetic complexity and statistics", Linear Algebra and its Applications 18(2):1253-1278, 1977.

Some supporting material

Check out our two-part monograph on Tensor Networks (Now Publishers, 2016, 2017)

A. Cichocki, D. Mandic, *et al.*



[Andrzej Cichocki, Danilo P. Mandic, Anh Huy Phan, Cesar F. Caiafa, Guoxu Zhou, Qibin Zhao, and Lieven De Lathauwer]

TENSOR DECOMPOSITIONS for Signal Processing Applications

[From two-way to multiway component analysis]

The widespread use of multisensor technology and the emergence of big data sets have highlighted the limitations of standard flat-view matrix models and the necessity to move toward more versatile data analysis tools. We show that higher-order tensors (i.e., multiway arrays) enable such a fundamental paradigm shift toward models that are essentially polynomial, the uniqueness of which, unlike the matrix methods, is guaranteed under very mild and natural conditions. Benefiting from the power of multilinear algebra as their mathematical backbone, data analysis techniques using tensor decompositions are shown to have great flexibility in the choice of constraints which match data properties and extract more general latent components in the data than matrix-based methods.

A comprehensive introduction to tensor decompositions is provided from a signal processing perspective, starting from the algebraic foundations, via basic canonical polyadic and Tucker models, to advanced cause-effect and multiview data analysis schemes. We show that tensor decompositions enable natural generalizations of some commonly used signal processing paradigms, such as canonical correlation and subspace techniques, signal separation, linear regression, feature extraction, and classification. We also cover computational aspects and point out how ideas from compressed sensing (CS) and scientific computing may be used for addressing the otherwise unmanageable storage and manipulation issues associated with big data sets. The

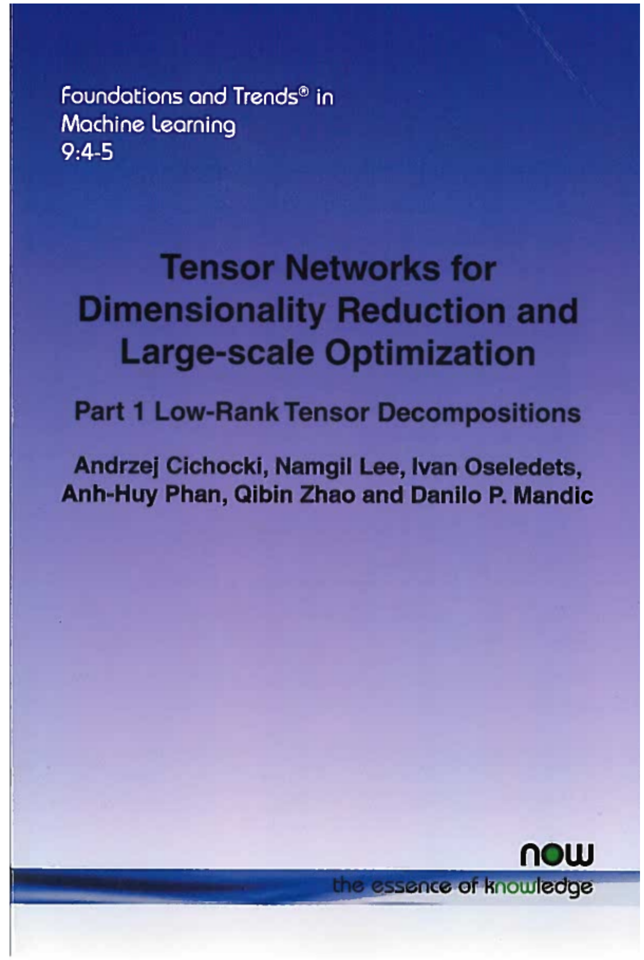
IMAGE LICENSED BY GRAPHIC STOCK

Digital Object Identifier 10.1109/MSP.2013.2297439
Date of publication: 12 February 2015

1053-5888/15©2015IEEE IEEE SIGNAL PROCESSING MAGAZINE [145] MARCH 2015

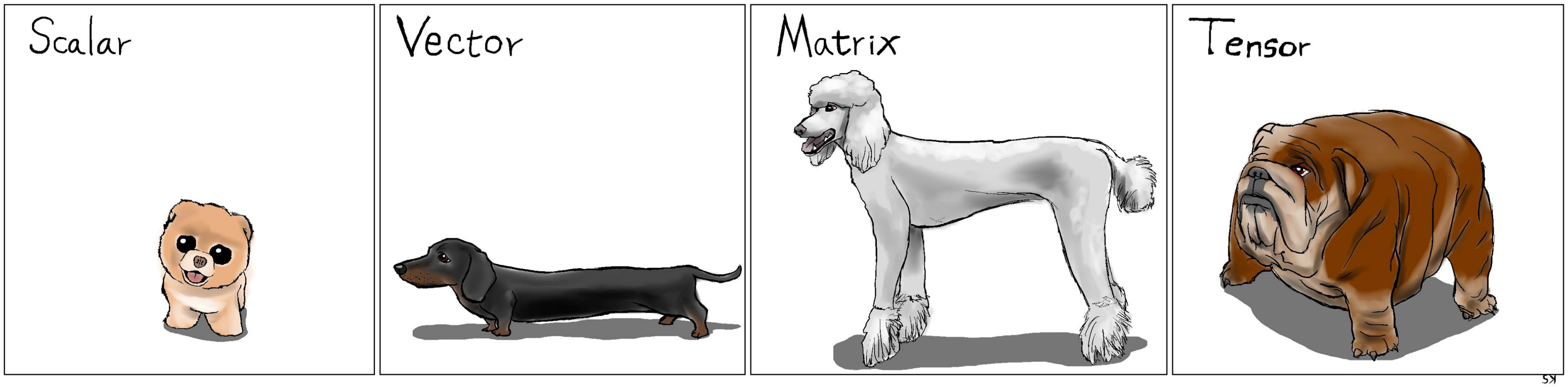
IEEE SPM, March 2015

A. Cichocki, D. Mandic, *et al.*



Foundations and Trends in Machine Learning, Parts 1 & 2

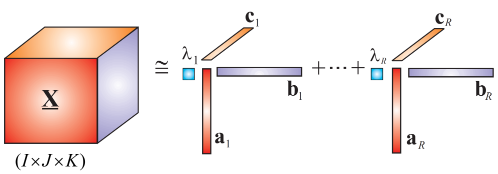
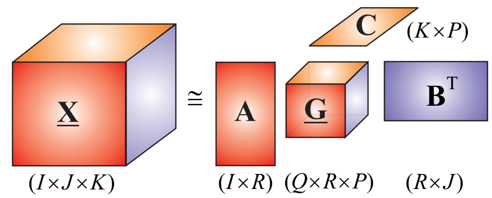
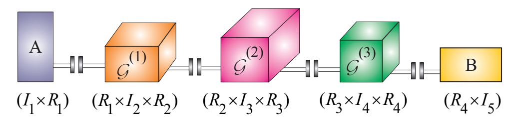
Thank you for your attention.



For the second part, please long onto the link

`www.github.com/IlyaKisil/inns-2019`

Comparison of multidimensional decompositions

CPD	Tucker	Tensor Train
		

storage complexity

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

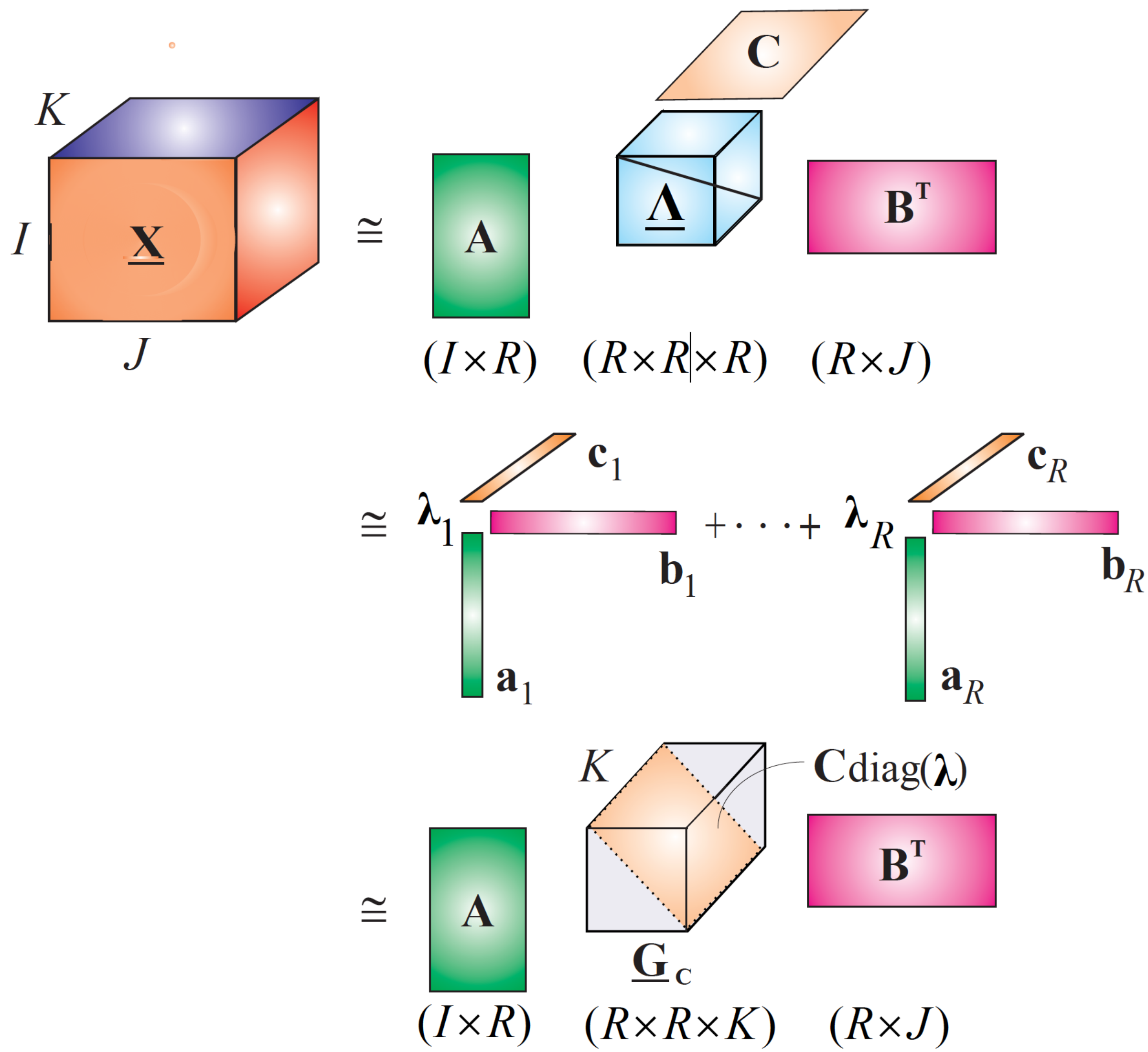
inherent structure

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

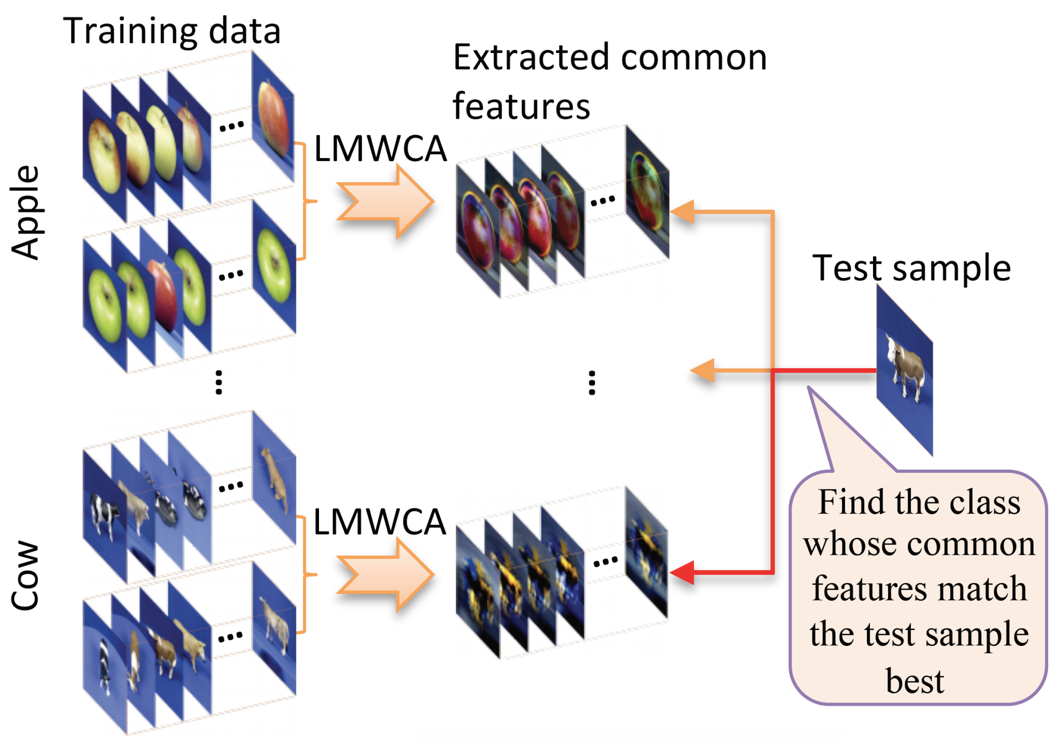
uniqueness conditions

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

Relation between the CPD and TKD
CPD = TKD with a diagonal core



Example 7: Linked Multiway Component Analysis (LMWCA) for classification applications

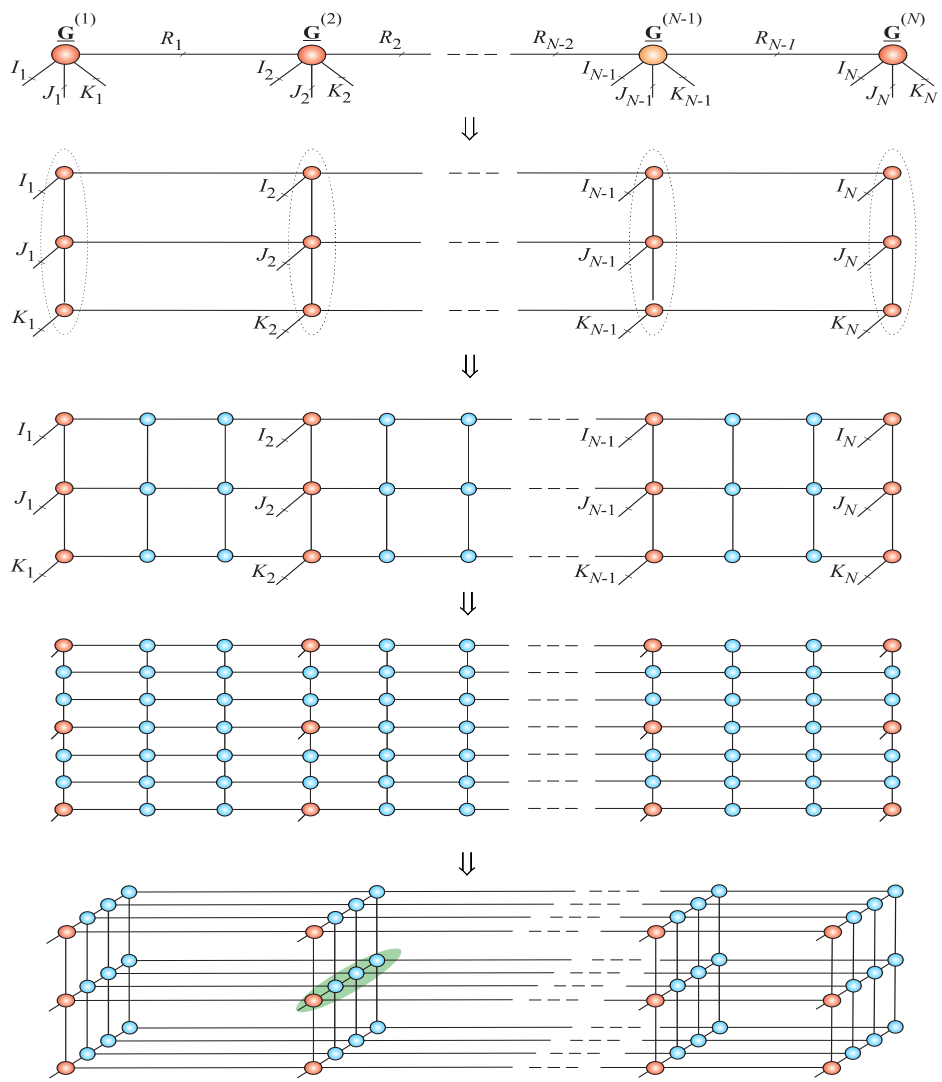


- Data fusion concerns the joint analysis of an ensemble of data sets
- Images of objects from different viewpoints can be grouped together and naturally linked as multi-block tensor data
- Such data blocks share common information, and at the same time this also allows for individual data features to be maintained
- An extracted set of common features is more discriminative ↪ better suited for classification

More complex tensor networks (TNs)

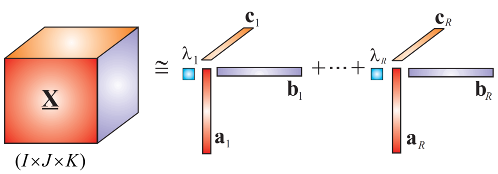
Representing a high order tensor as a set of matrices and lower order tensors

- The number of edges on any core tensor represents its order
- The number of free edges of the TN represent the order of the tensor being represented
- TNs have the main advantages of
  - being suited to deal with the curse of dimensionality
  - performing inherent feature extraction
- 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)

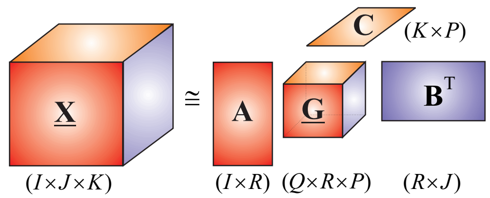


Comparison of multidimensional decompositions

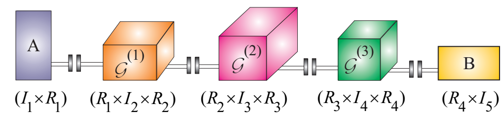
CPD



Tucker



Tensor Train



storage complexity

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

inherent structure

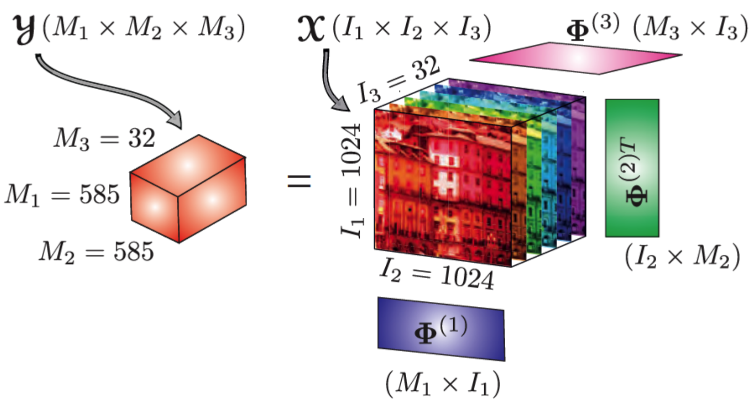
CPD	Tucker	Tensor Train
Represented through rank-1 terms	Represented through core tensors and factor matrices	Represented through tensor contractions

uniqueness conditions

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

Example 9: Higher-order compressed sensing

Kronecker-CS of a 32-channel hyperspectral image $\mathcal{X}$



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

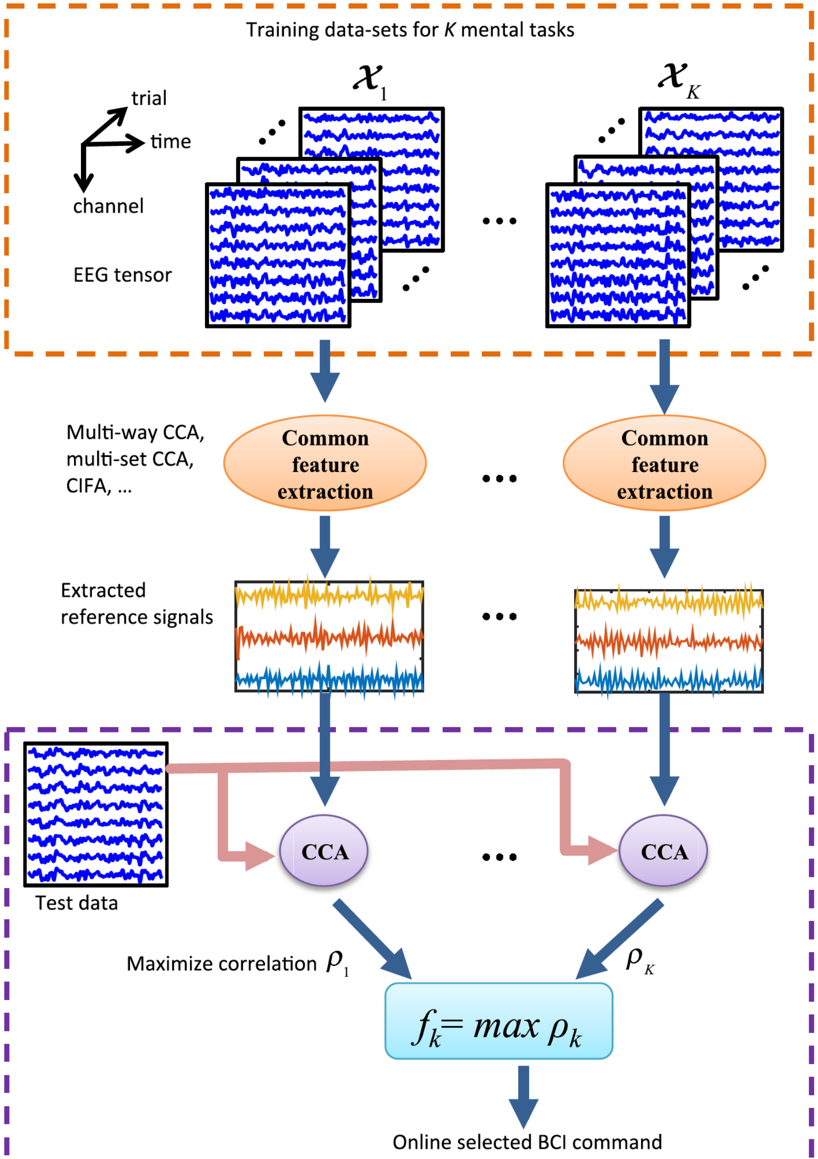
Original hyperspectral image - RGB display

(1024 x 1024 x 32) (256 x 256 x 32)

Reconstruction (SP=33%, PSNR = 35.51dB) - RGB display

(1024 x 1024 x 32) (256 x 256 x 32)

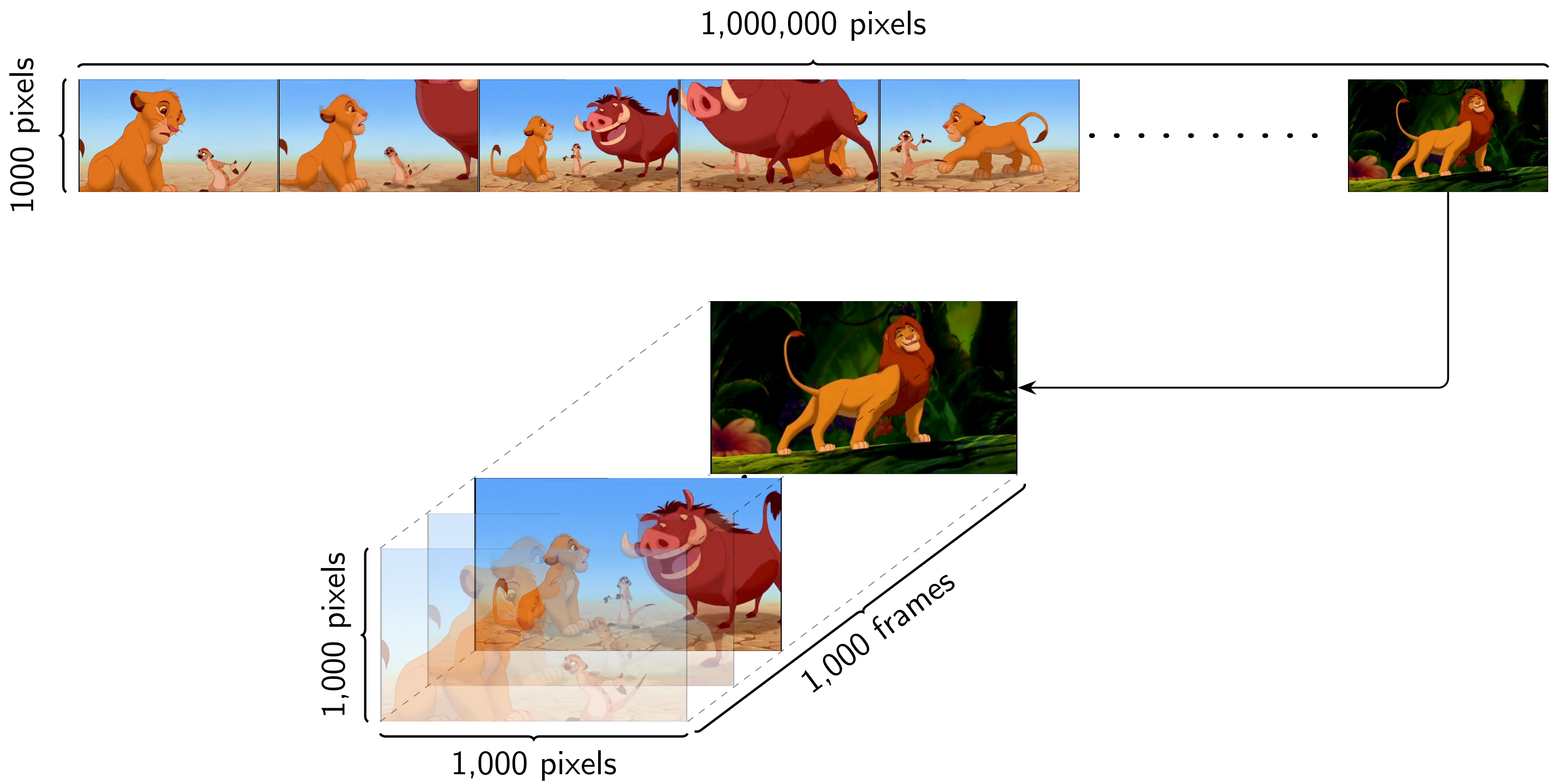
Example 8: SSVEP recognition in EEG based on Linked Multiway Component Analysis (LMWCA)



- Steady-state visual evoked potentials (SSVEP) are periodic neural responses in EEG, which are elicited at the same frequency as a blinking visual stimulus
- EEG data recorded at the same stimulus frequency should share some common features, reflecting this frequency information
- Such common features extracted from EEG bear real SSVEP characteristics ↬ more qualified as references for SSVEP recognition
- The LMWCA identifies and separates the common and individual features from multi-block tensor data, and can be a very effective tool for solving classification problems
- The LMWCA ignores variances of common components ↬ weak features can be detected

Example 9a: Tensor construction from a video clip

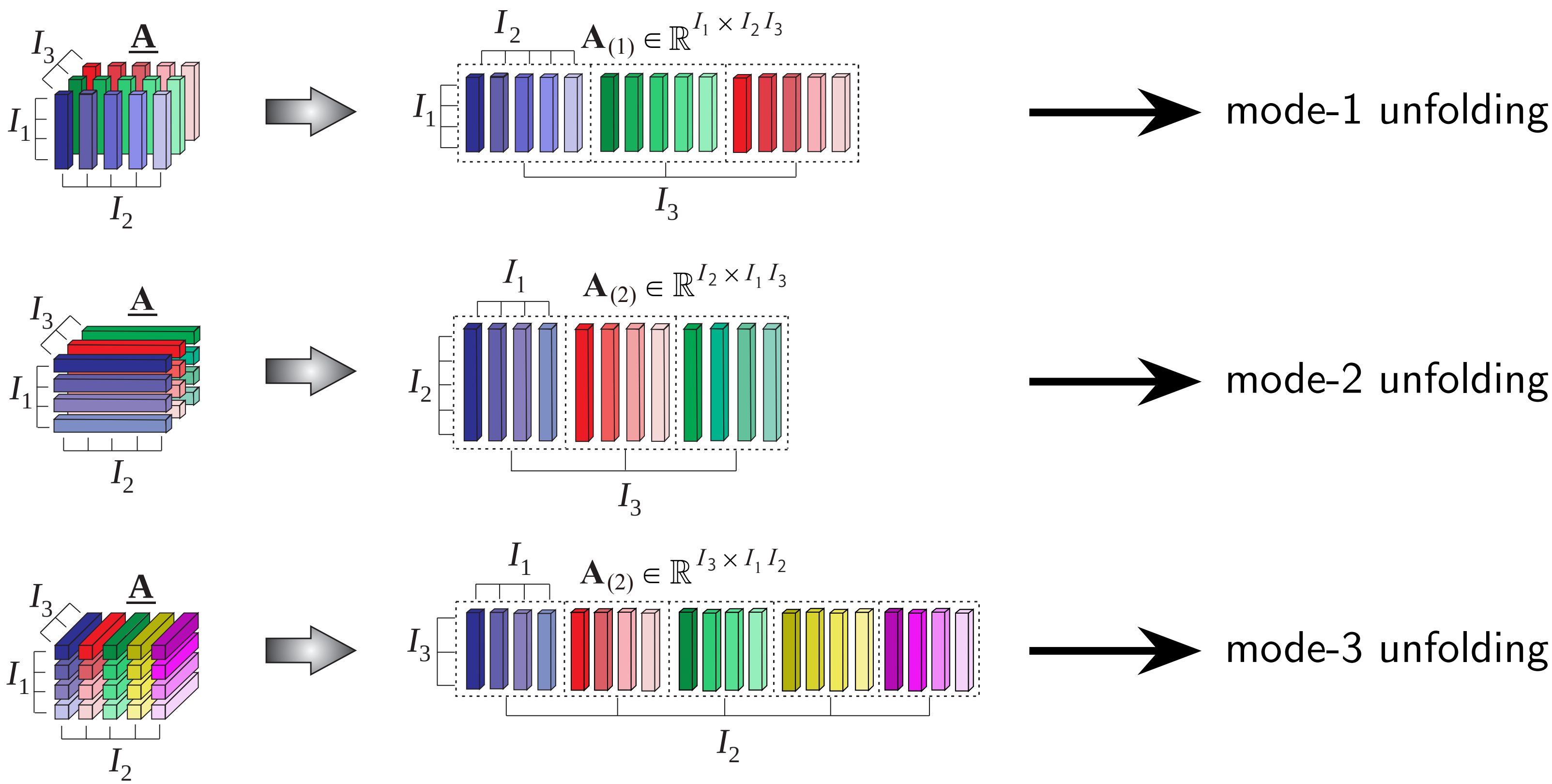
↬ pixel$_X$ × pixel$_Y$ × frame



- 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

Unfolding of a tensor in different modes

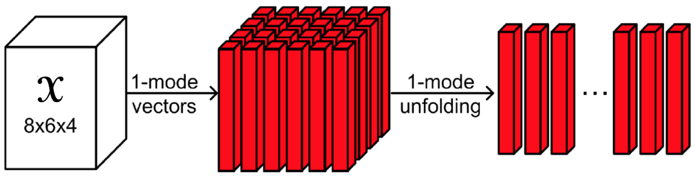
Converts a higher-order tensor into a smaller tensor, matrix, or vector



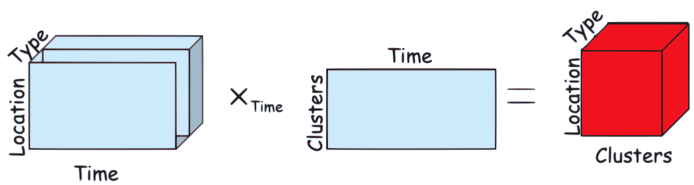
- This operation maps tensor entries into a matrix, in e.g. a 'slice-by-slice' manner
- Such flattening (unfolding) prior to data analysis breaks the inherent structure in data and obscures latent dependencies between the modes

Multilinear operations and definitions

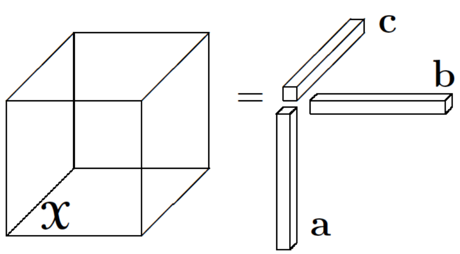
Mode-n unfolding



Mode-n product



Outeproduct



- The order of a tensor is a number of dimensions $\underline{\mathbf{X}} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$
- The mode-n unfolding of a tensor:

$$\underline{\mathbf{X}} \rightarrow \mathbf{X}_{(n)}$$

- The mode-n product:

$$\underline{\mathbf{Y}} = \underline{\mathbf{X}} \times_n \mathbf{U} \Leftrightarrow \mathbf{Y}_{(n)} = \mathbf{U}\mathbf{X}_{(n)}$$

- The outer product of N vectors results in a rank-1 tensor of order N:

$$\mathbf{a}_1 \circ \mathbf{a}_2 \circ \cdots \circ \mathbf{a}_N = \underline{\mathbf{X}} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$$

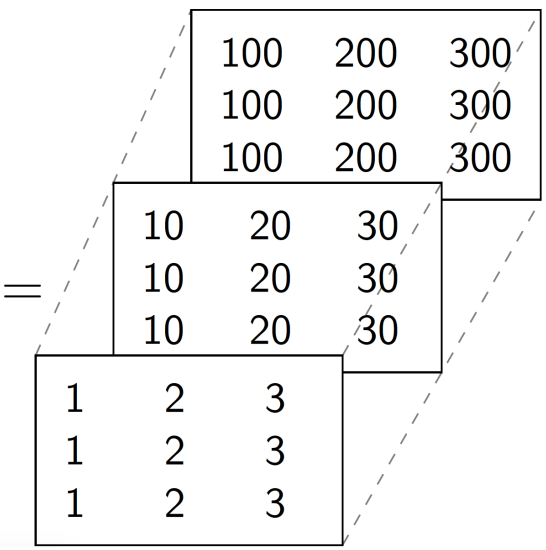
Example 9: The outer product in three dimensions

Consider the vectors $\mathbf{a} = [1 \quad 1 \quad 1]^T, \mathbf{b} = [1 \quad 2 \quad 3]^T, \mathbf{c} = [1 \quad 10 \quad 100]^T$.

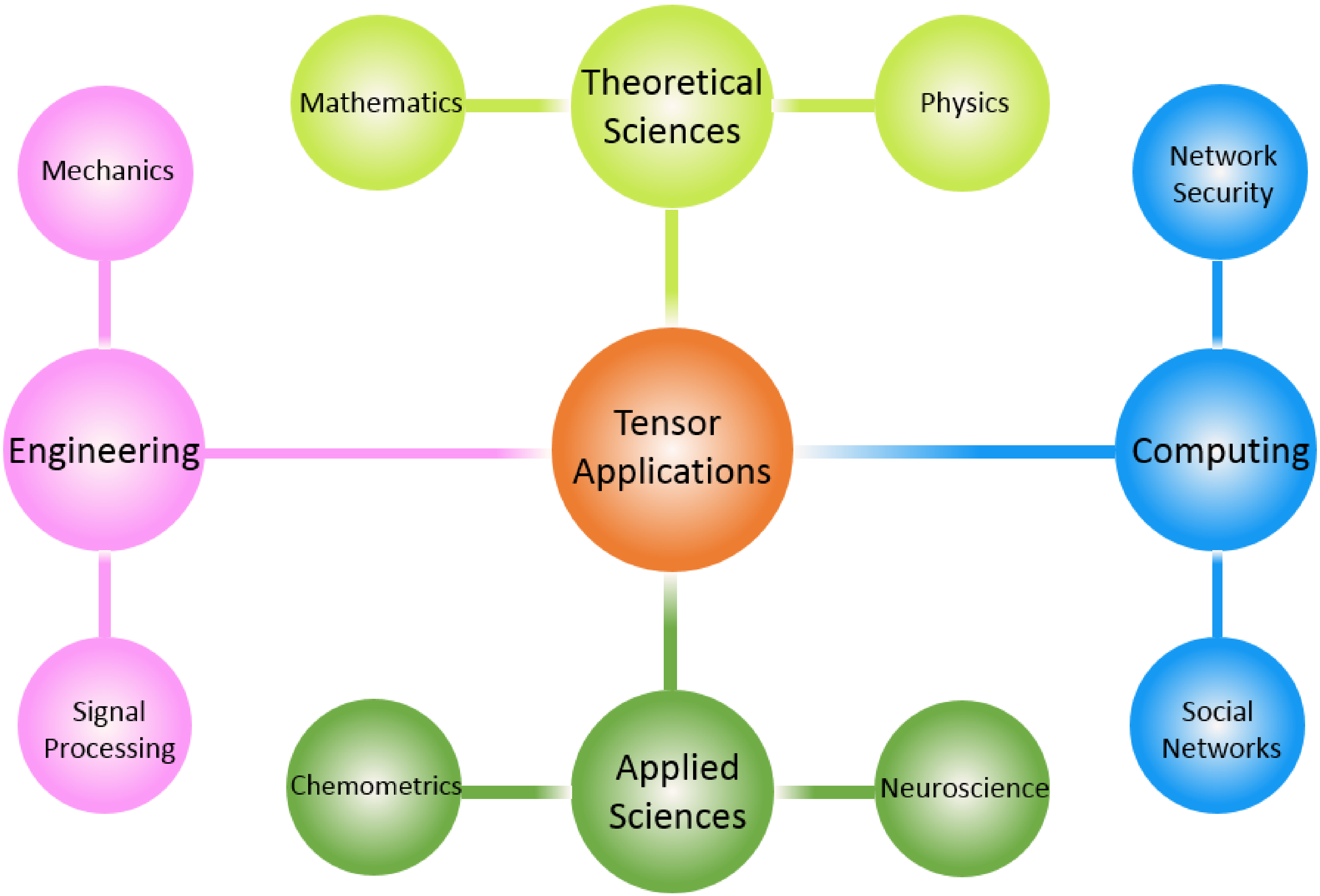
$$\mathbf{a} \circ \mathbf{b} \circ \mathbf{c} = \textbf{?} \tag{3}$$

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

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

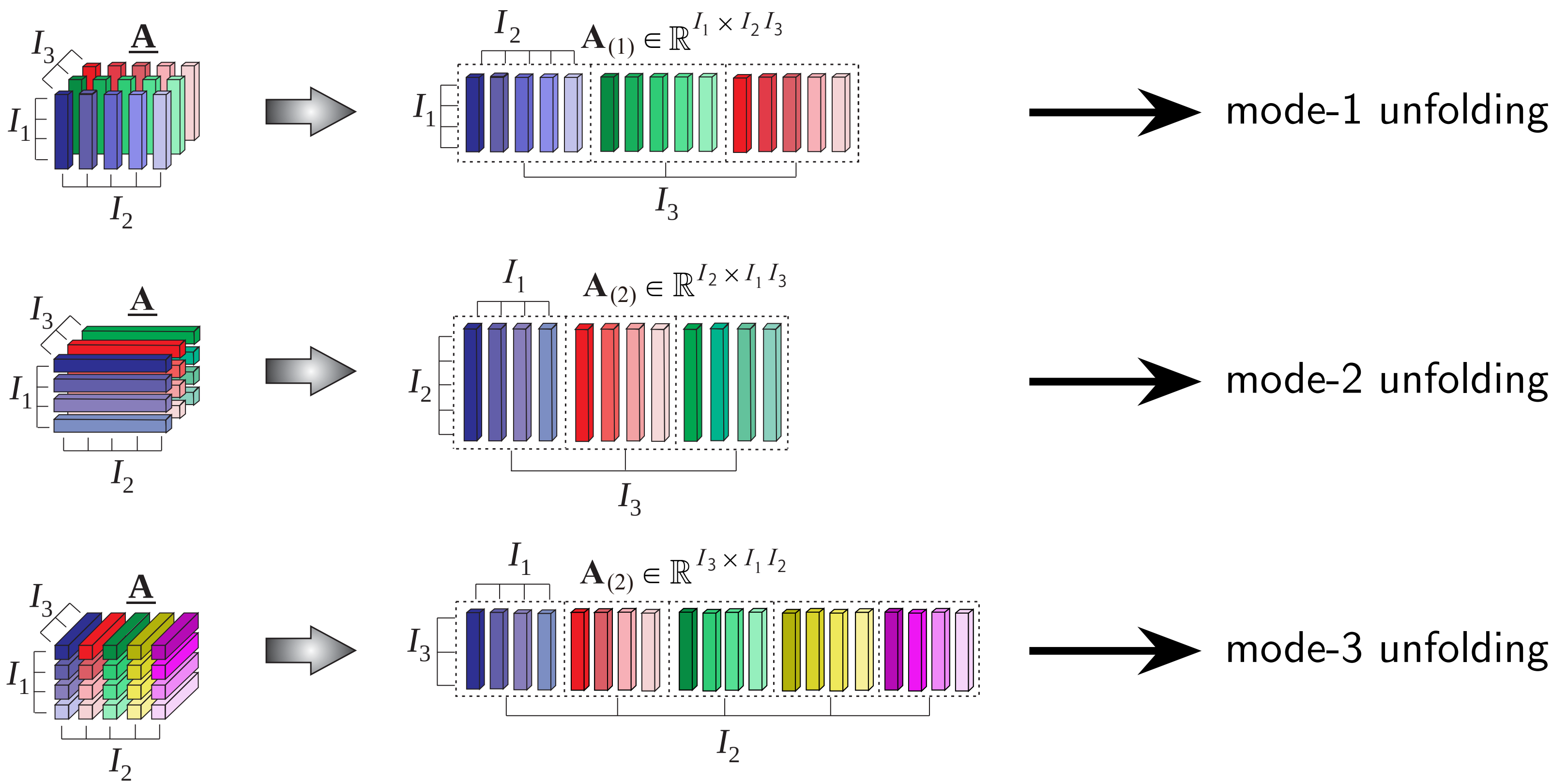


Tensors $\looparrowright$ ability to maintain original data structure, and to perform high-level feature extraction



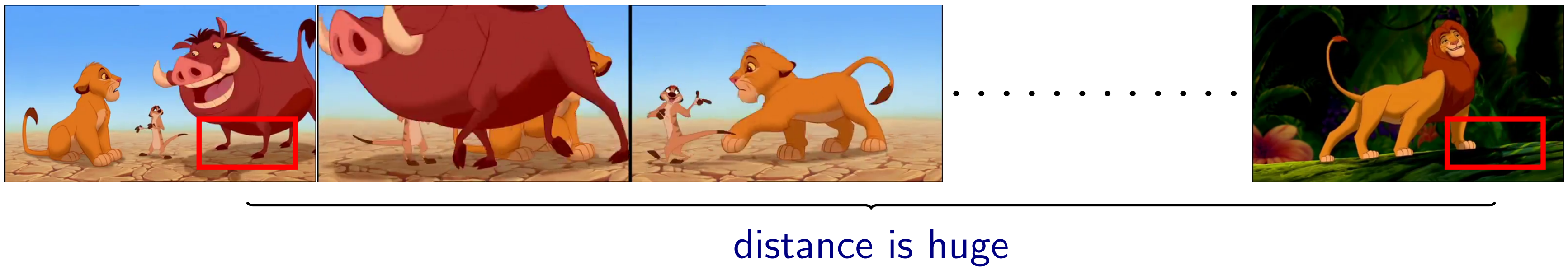
Unfolding of a tensor in different modes

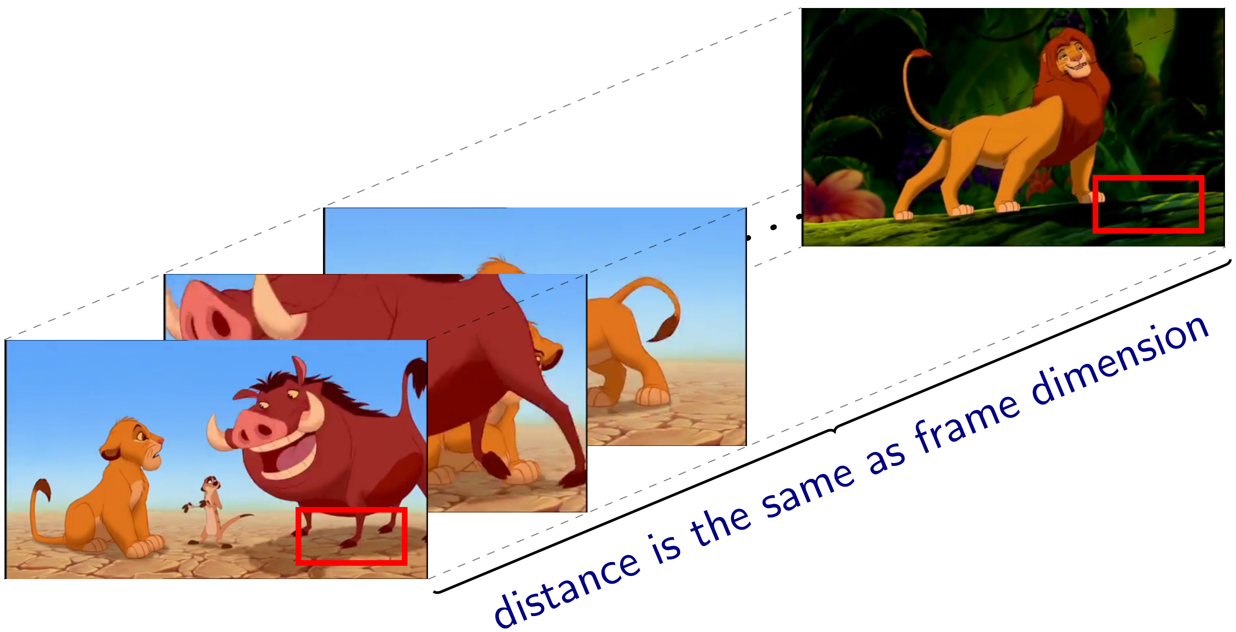
Converts a higher-order tensor into a smaller tensor, matrix, or vector



- 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

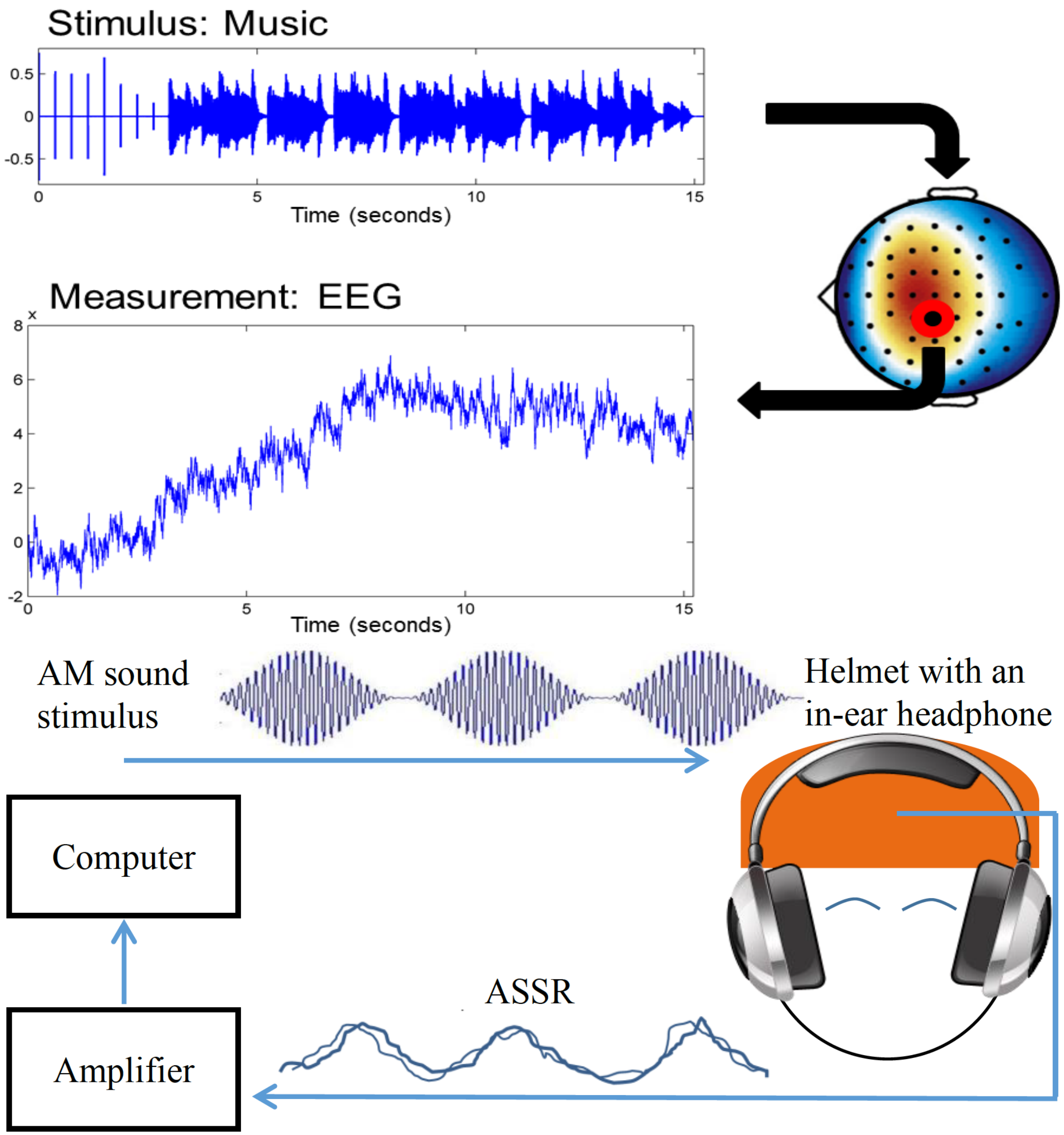
Example 10: Video clip $\looparrowright$ compact tensor representation





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.

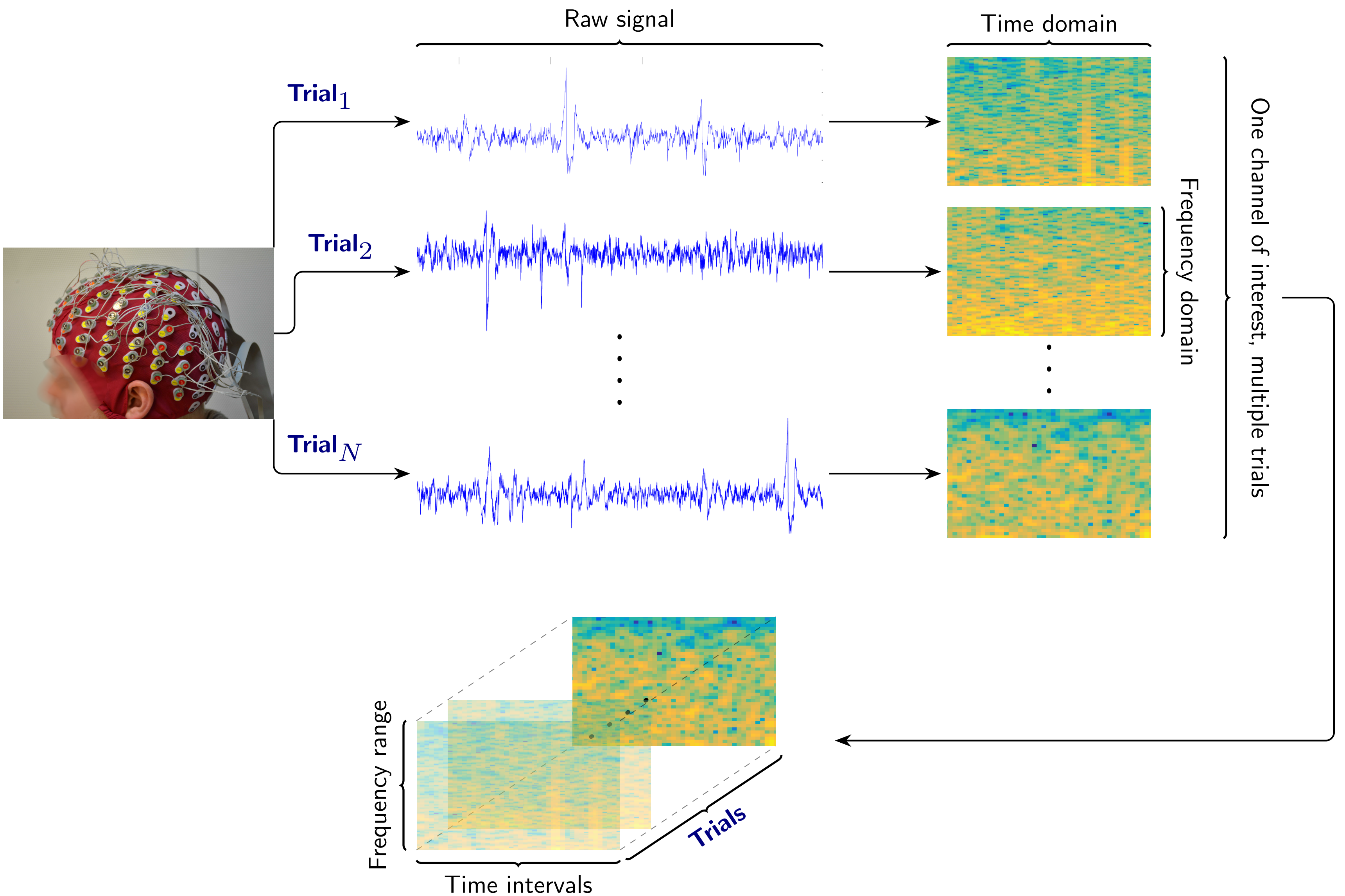
Tensorisation: Multi-way representation of multichannel biomedical data



- 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 therefore inherently multi-dimensional (many channels), and multi-way

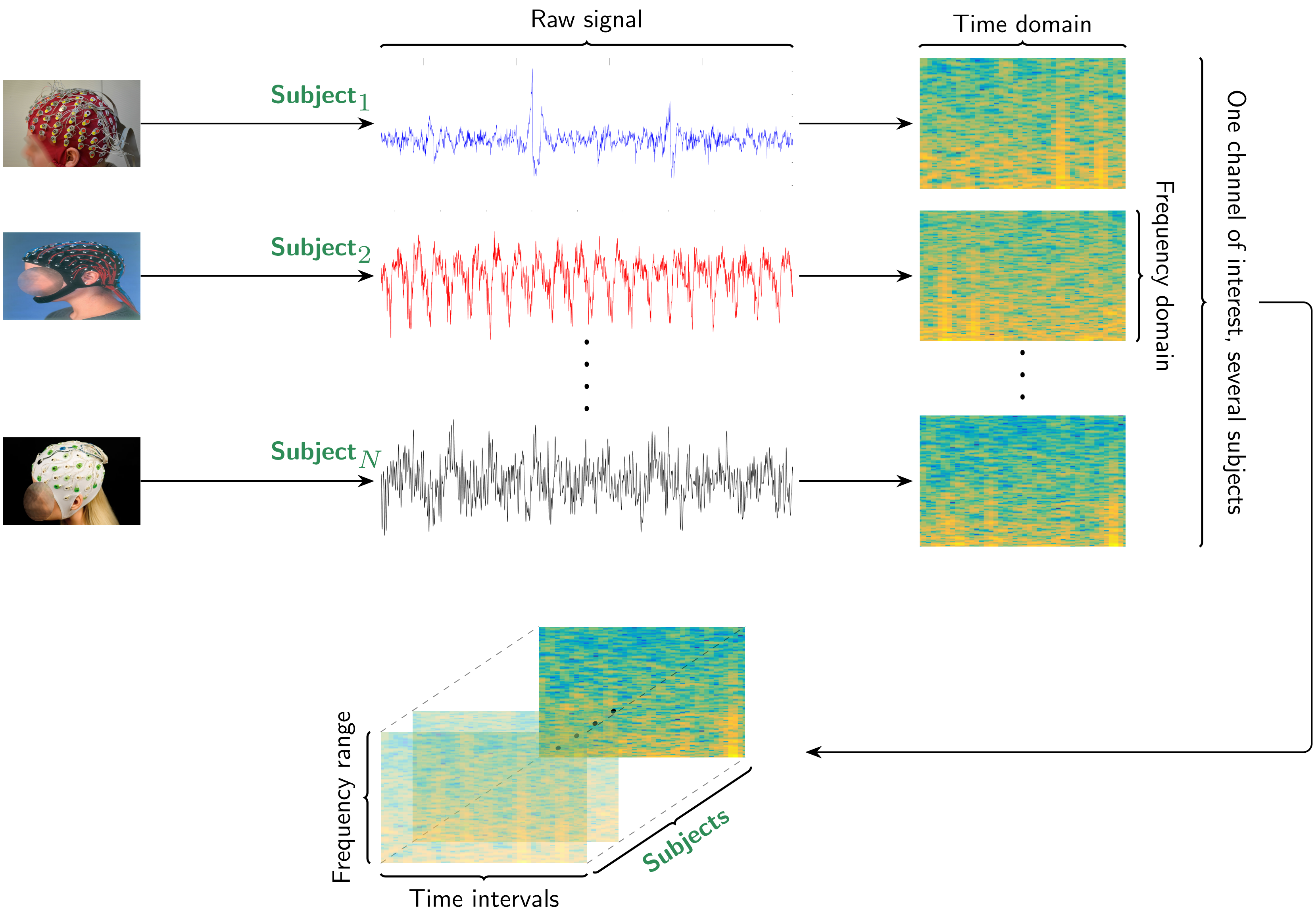
Example 11b: Tensor construction from different trials

↬ trial × frequency × time

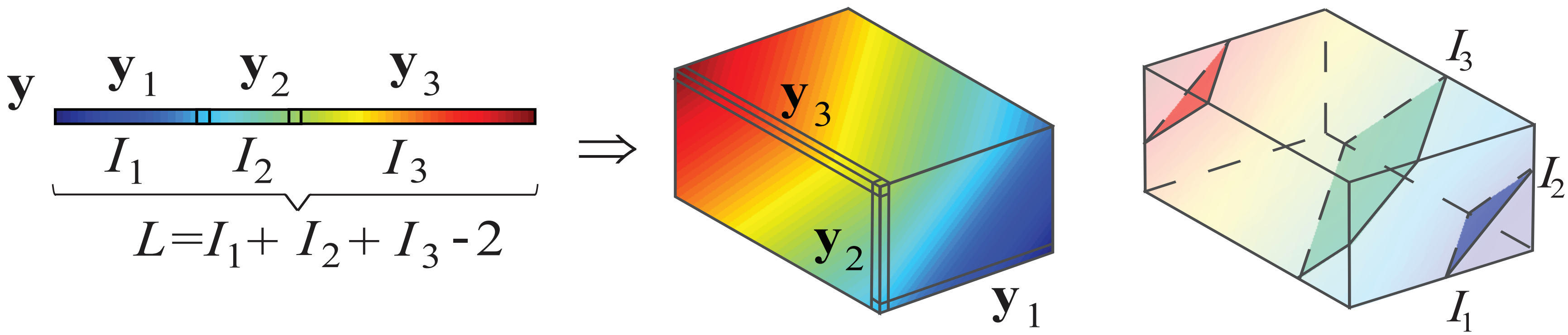


Example 11c: Tensor construction from different subjects

↬ subject × frequency × time



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

$$\begin{bmatrix} a & az & az^2 & az^3 & \cdots \end{bmatrix} \qquad (4)$$

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

$$\mathbf{H} = \begin{bmatrix} a & az & az^2 & \cdots \\ az & az^2 & az^3 & \cdots \\ az^2 & az^3 & az^4 & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix} = a \begin{bmatrix} 1 \\ z \\ z^2 \\ \vdots \end{bmatrix} \begin{bmatrix} 1 & z & z^2 & \cdots \end{bmatrix} = a\, \mathbf{z} \circ \mathbf{z} \qquad (5)$$

- 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 of two vectors, $\mathbf{x}$ and $\mathbf{y}$, of respective lengths I and $L > I$, given by

$$\mathbf{z} = \mathbf{x} * \mathbf{y} \tag{6}$$

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

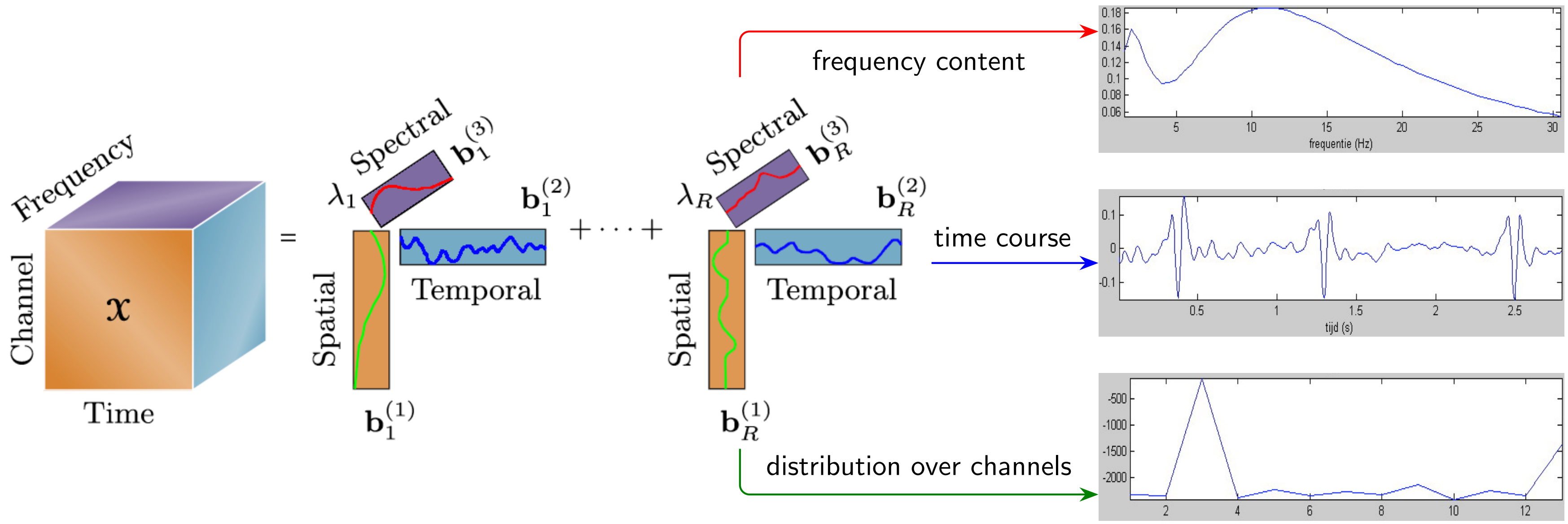
$$\mathbf{z}_{I:L} = \mathbf{Y}^T\mathbf{x} = \begin{bmatrix} y(I) & y(I-1) & y(I-2) & \cdots & y(1) \\ y(I+1) & y(I) & y(I-1) & \cdots & y(2) \\ y(I+2) & y(I+1) & y(I) & \cdots & y(3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y(L) & y(L-1) & y(L-2) & \cdots & y(J) \end{bmatrix} \begin{bmatrix} x(1) \\ x(2) \\ x(3) \\ \vdots \\ x(I) \end{bmatrix} \tag{7}$$

- 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

$$\mathbf{z} = \mathbf{x}_1 * \mathbf{x}_2 * \mathbf{y} \tag{8}$$

- First, a Toeplitz matrix $\mathbf{Y}$ is obtained from $\mathbf{x}_1 * \mathbf{x}_2$ as shown in Eq. (7)
- 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 $\underline{\mathbf{Y}} = [\mathbf{Y_1}, \ldots, \mathbf{Y_J}]$

Intuition and physical meaning behind the CPD



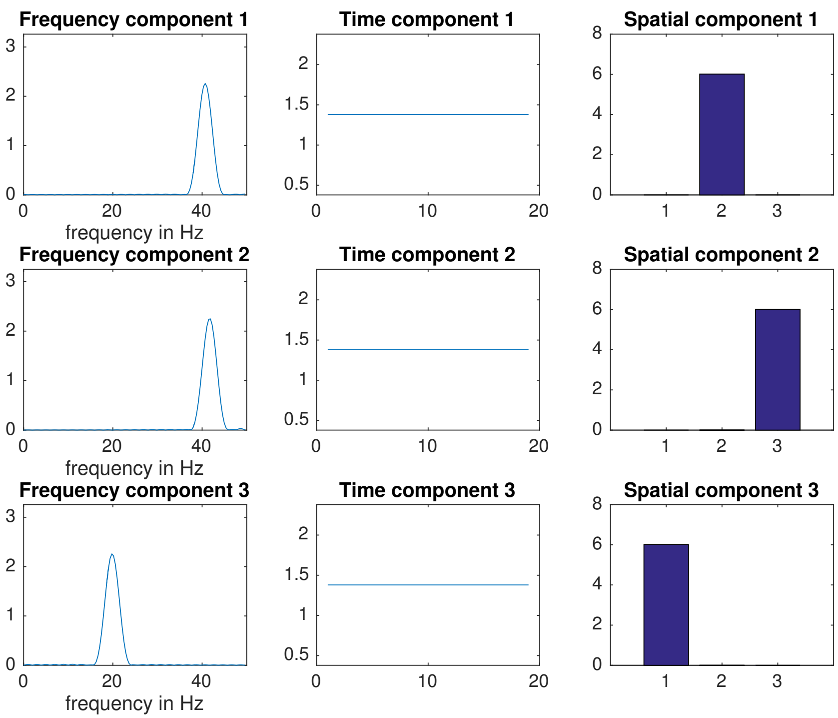
- Components $\mathbf{b}_i^{(1)}, \mathbf{b}_i^{(2)}, \mathbf{b}_i^{(3)}$ (factor 1) are associated with one another (linked)
- However, none of them is associated with any other set of such components (factors) for $i \neq j$, e.g. with $\mathbf{b}_R^{(1)}, \mathbf{b}_R^{(2)}, \mathbf{b}_R^{(3)}$
- 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

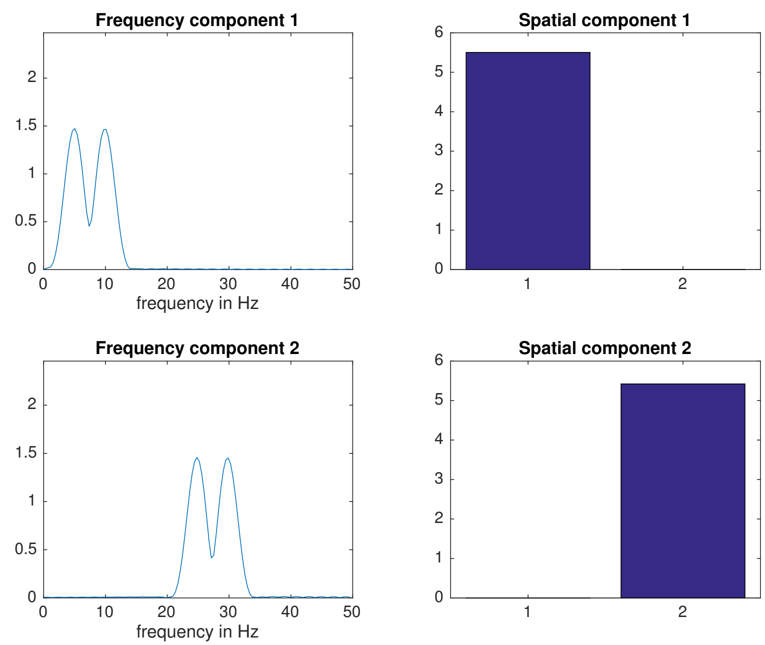
$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \lambda_r \cdot \mathbf{b}_r^{(1)} \circ \mathbf{b}_r^{(2)} \circ \mathbf{b}_r^{(3)} = [\![\underline{\mathbf{D}}; \mathbf{B}^{(1)}, \mathbf{B}^{(2)}, \mathbf{B}^{(3)}]\!] \qquad (9)$$

Intuition and physical meaning behind the CPD

$$
\begin{aligned}
1 &= 1020 \\
2 &= 1041 \\
3 &= 1042
\end{aligned}
\tag{10}
$$

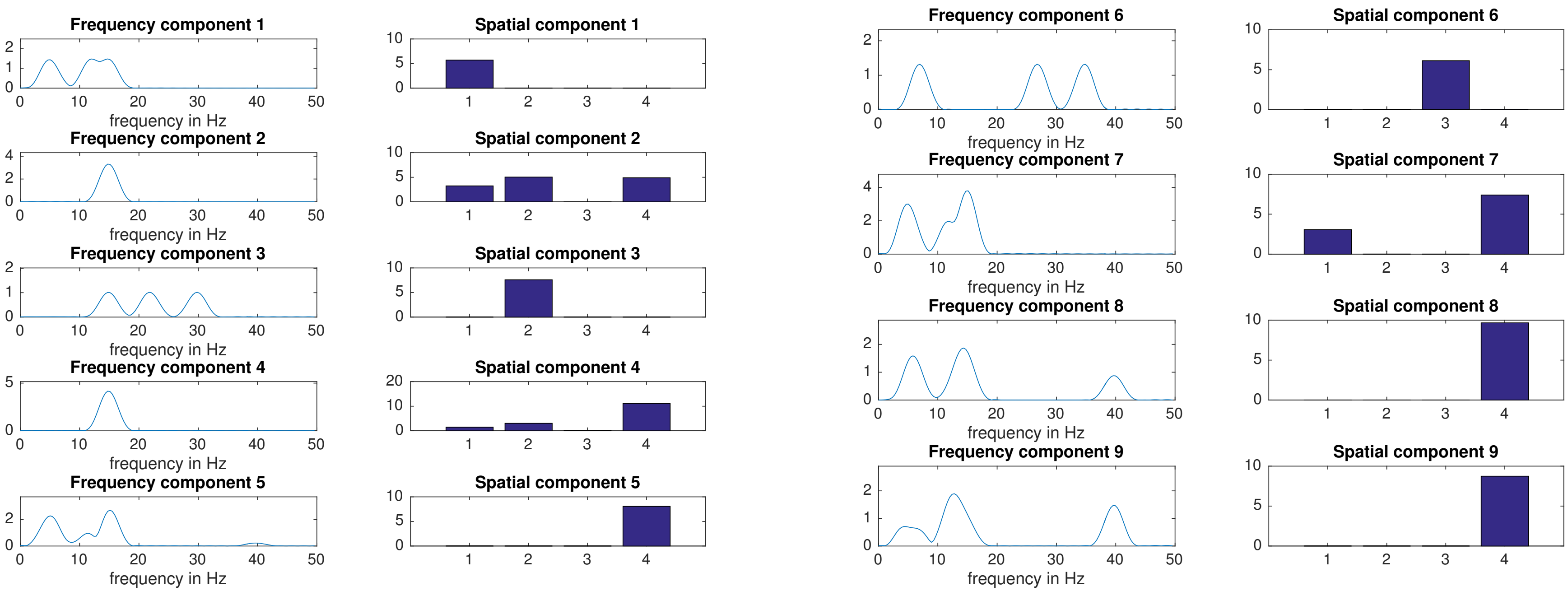
$$
\begin{aligned}
1 &= 105 + \\
&\quad 1010 \\
2 &= 1025 + \\
&\quad 1030
\end{aligned}
\tag{11}
$$





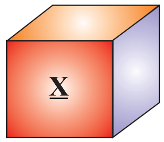
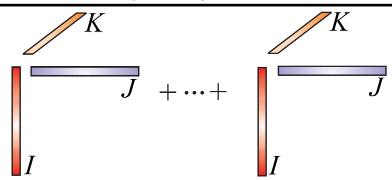
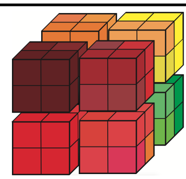
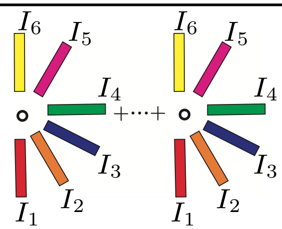
Intuition and physical meaning behind the CPD

$$1 = 105 + 1012 + 1015$$
$$2 = 1015 + 1022 + 1030$$
$$3 = 107 + 1027 + 1035 \qquad (12)$$
$$4 = 106 + 1013 + 1040$$



Super-compression inherent to CPD

Exponential complexity for the raw data format ⇝ linear complexity for TDs

Data format	length(mode$_n$)=10	length(mode$_n$)=10^m	General case
 $(I \times J \times K)$	10^3	10^{3m}	IJK
	$R \cdot 3 \cdot 10$	$R \cdot 3 \cdot 10^m$	$R(I+J+K)$
 $(I_1 \times I_2 \times I_3 \times I_4 \times I_5 \times I_6)$	10^6	10^{6m}	$\prod_{n=1}^{6} I_n$
	$R \cdot 6 \cdot 10$	$R \cdot 6 \cdot 10^m$	$R \sum_{n=1}^{6} I_n$

Number of elements in a data format

- R is the rank of a tensor $\underline{\mathbf{X}}$ ↬ CPD is a sum of R rank-1 terms. On practice $R \ll I_n$
- For an N^{th}-order tensor all I^N elements are efficiently represented through the CPD as a linear (instead of exponential) function of number of elements in each mode

Notes

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