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)
- Tensor networks and their applications

Big data processing $\not\hookrightarrow$ 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 ~ 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 $= 2$ $\not\hookrightarrow 10^{15}$ 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 $\not\hookrightarrow$ **to make sense from Big Data**?

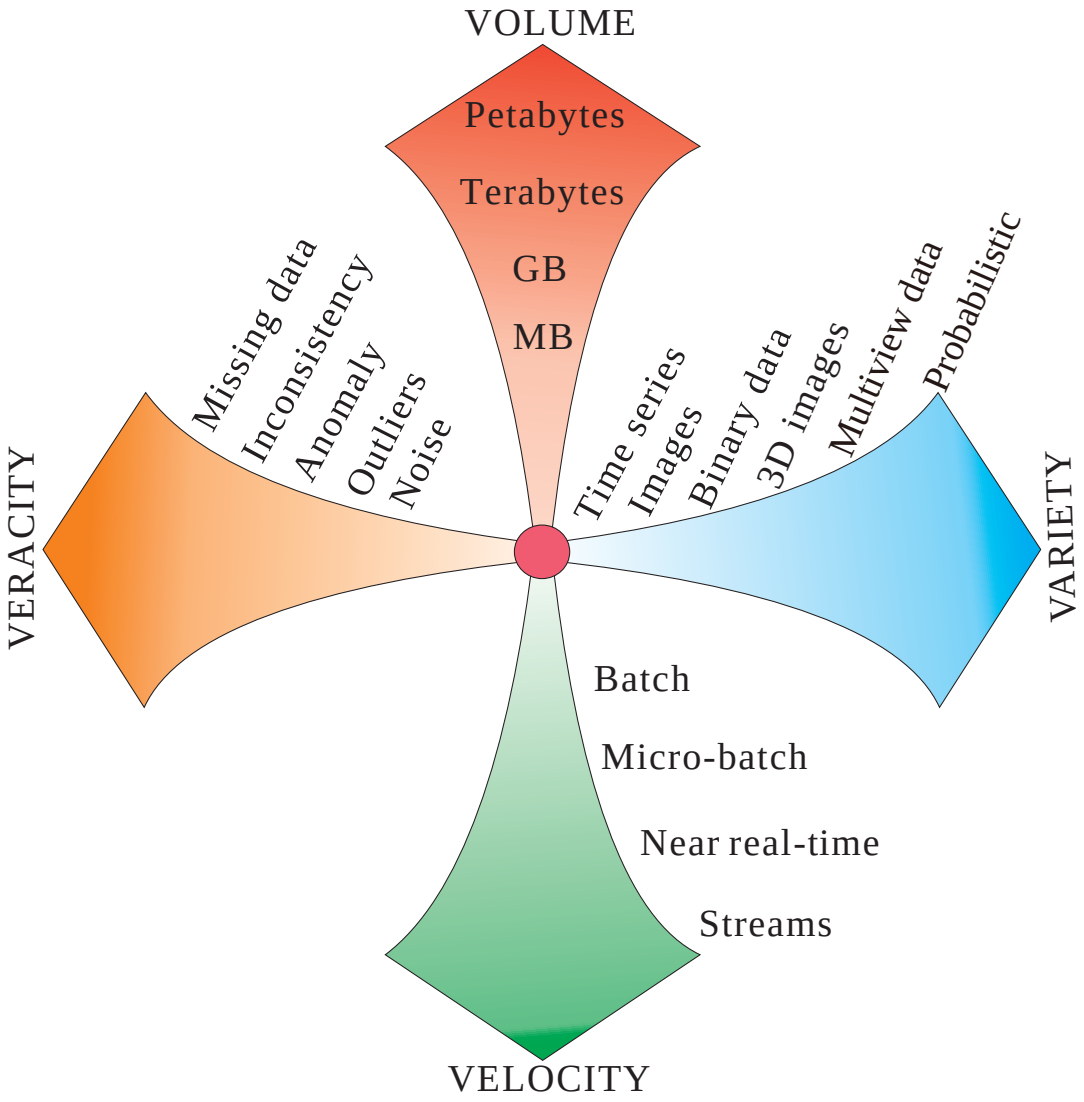
Some facts about Big Data opportunities

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), ...

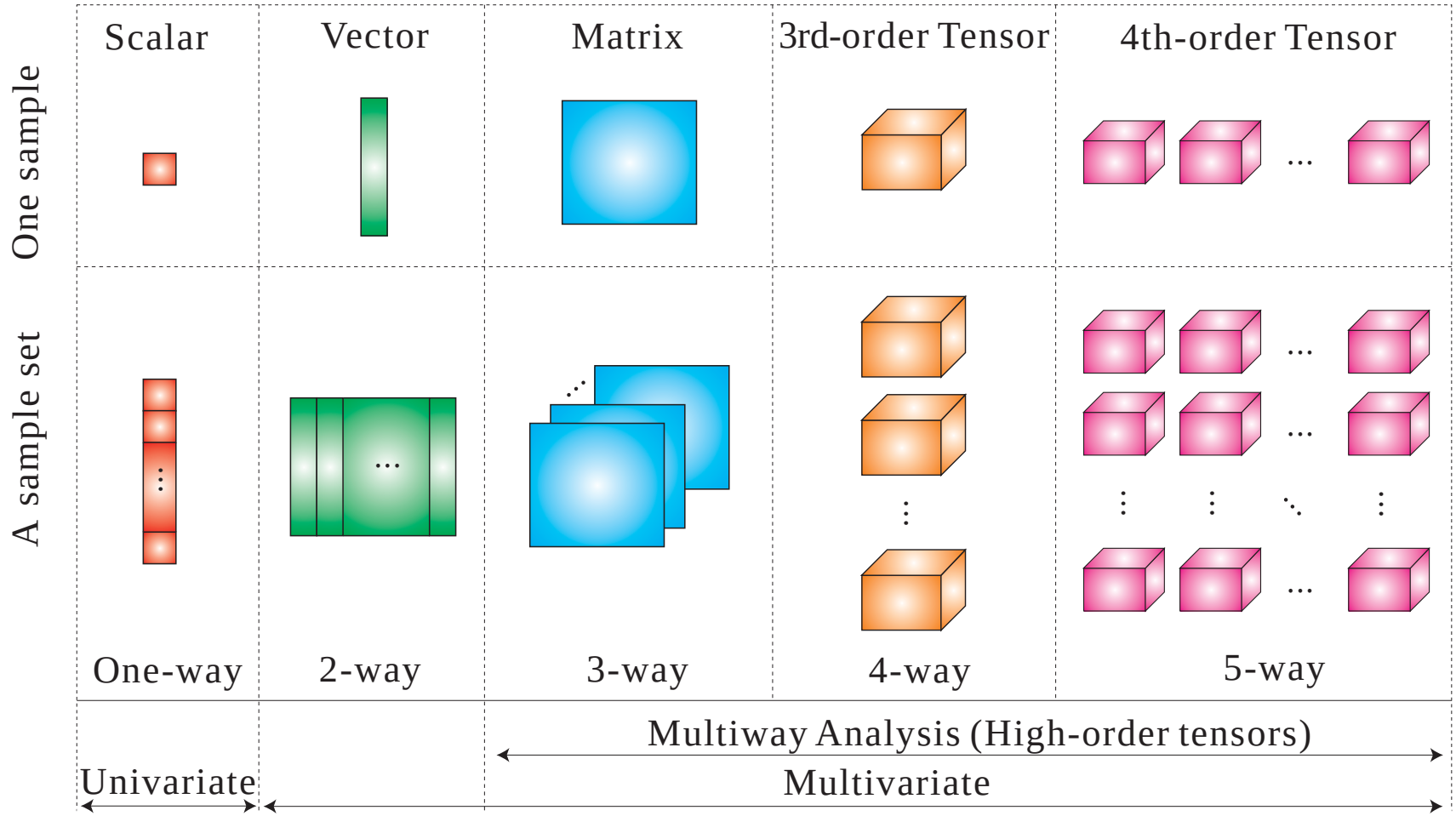


Signal processing an machine learning for big data
Challenges and opportunities

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

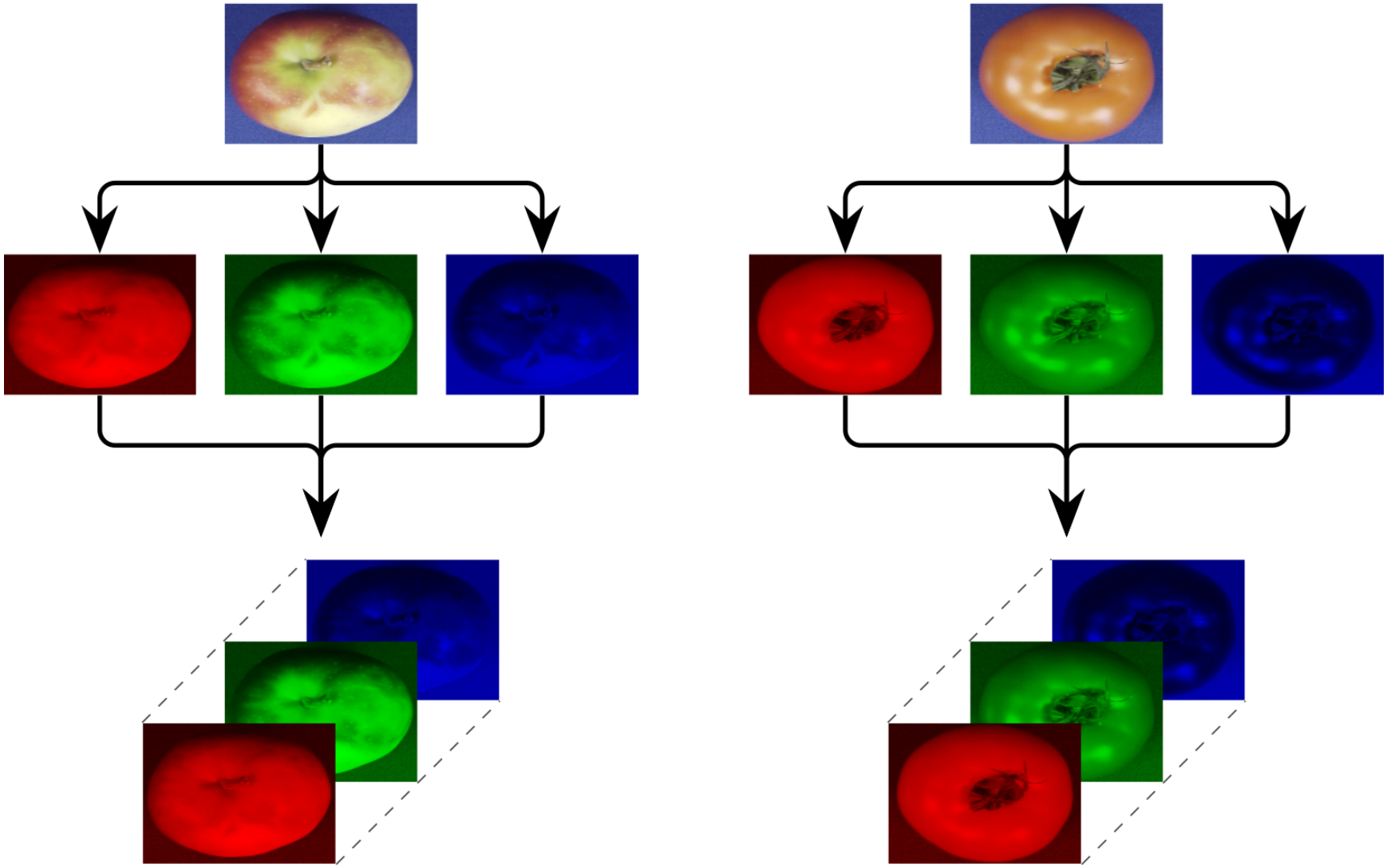
Types of data: From a scalar to a tensor



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

RGB image as a tensor $\looparrowright$ Tensor construction

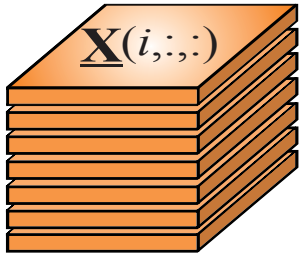
$\looparrowright$ pixel$_X$ $\times$ pixel$_Y$ $\times$ base color



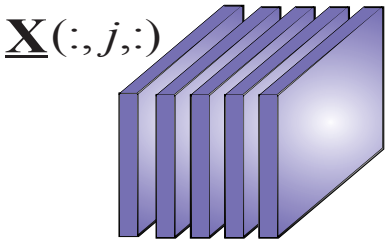
Sub-structures within tensors

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

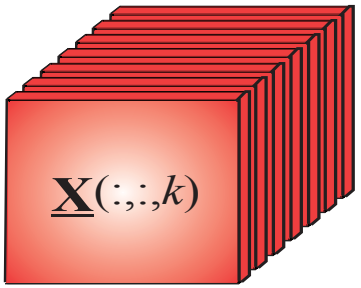
Horizontal Slices



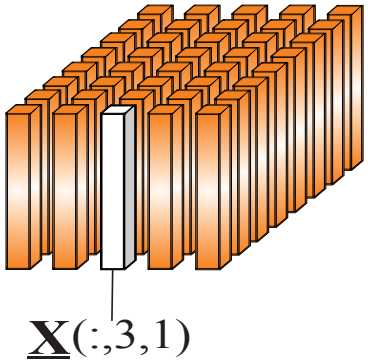
Lateral Slices



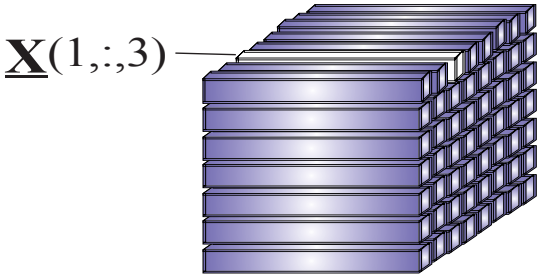
Frontal Slices



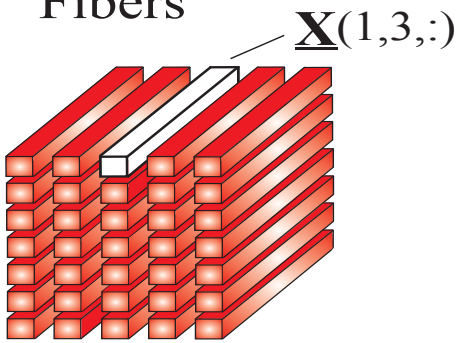
Column (Mode-1) Fibers



Row (Mode-2) Fibers



Tube (Mode-3) Fibers

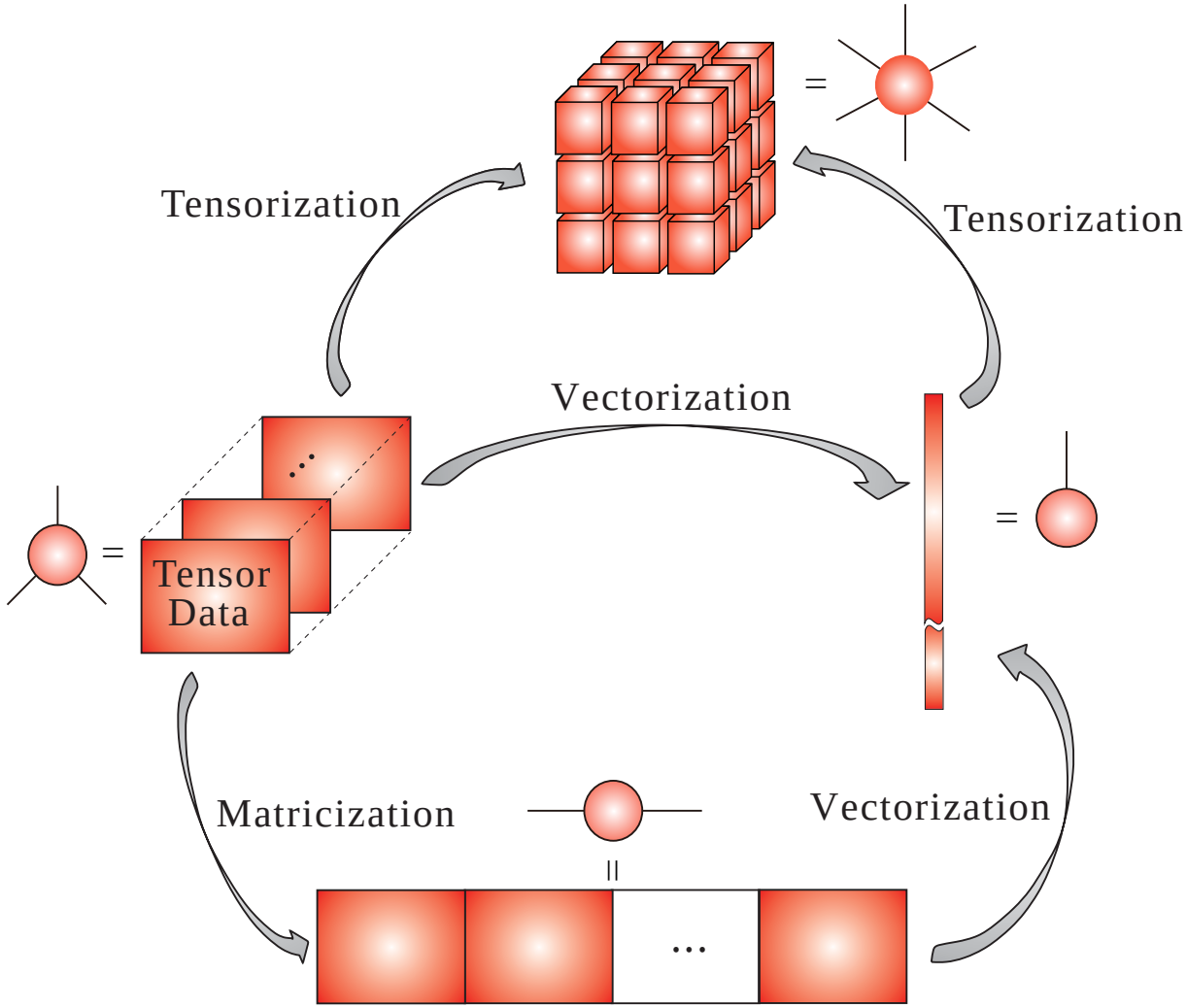


☞ A fiber is produced by fixing two indices and varying one, e.g. $\underline{\mathbf{X}}(1,3,:)$

Reshaping of data structures: General concept

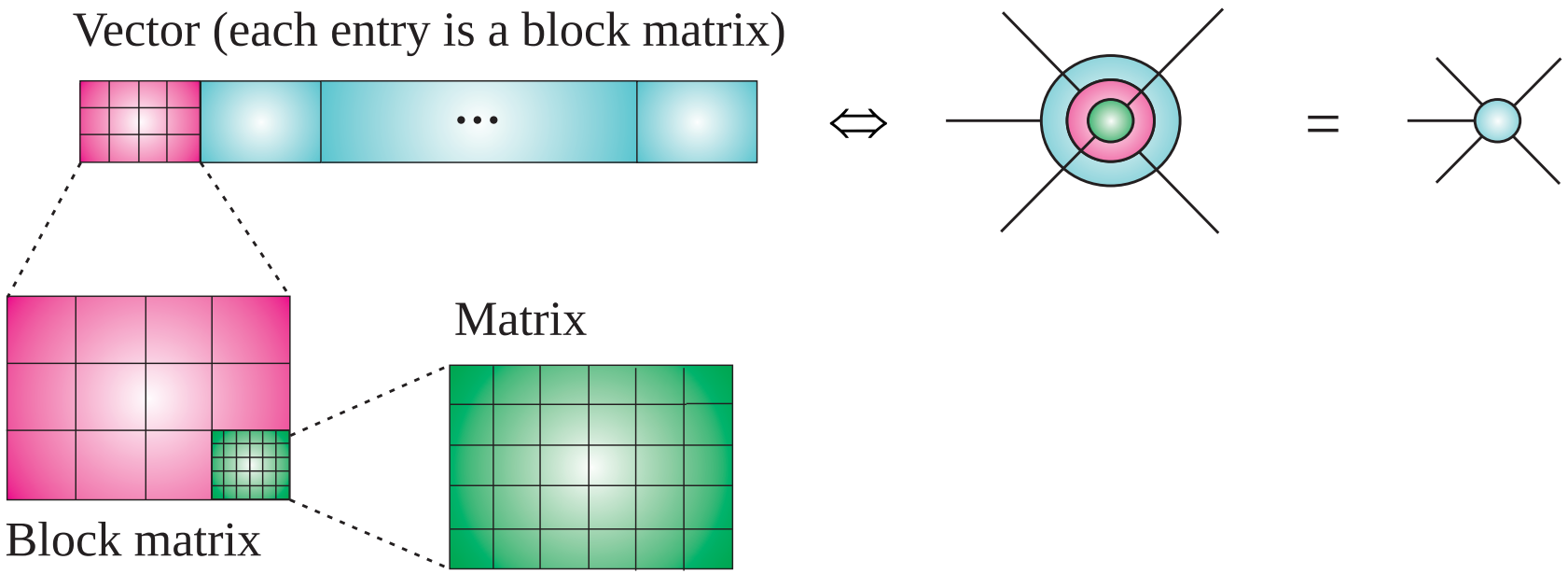
Vector, matrix or small-scale tensor $\hookrightarrow$ higher-order tensor is referred to as folding

- 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.



Further tensor network notation

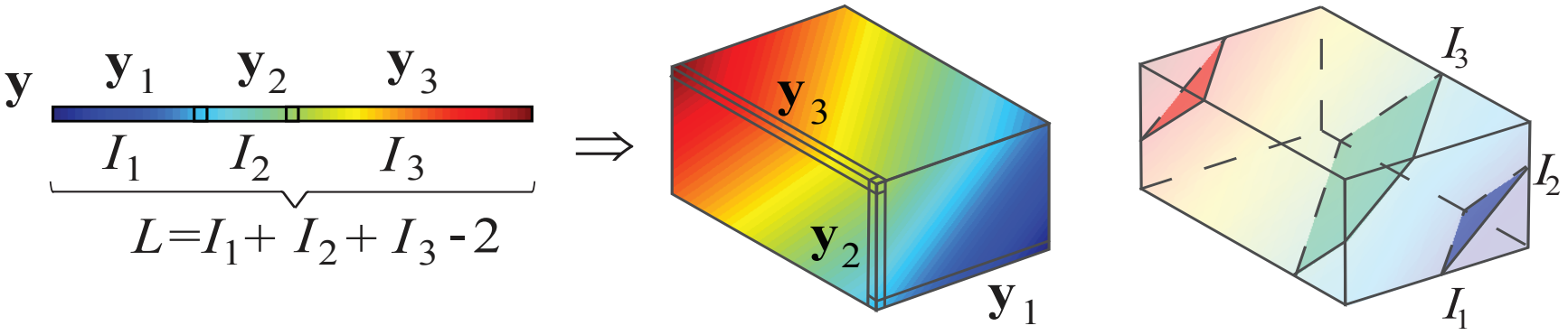
Compact representation for even most complicated operations



- In addition, TNs have the advantage of offering very efficient and intuitive ways to visualise tensors

- For example, a 5-th order tensor could be interpreted as a vector of block matrices, as shown in the figure above.

Deterministic folding techniques for structured data ↬ Hankel folding operator



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

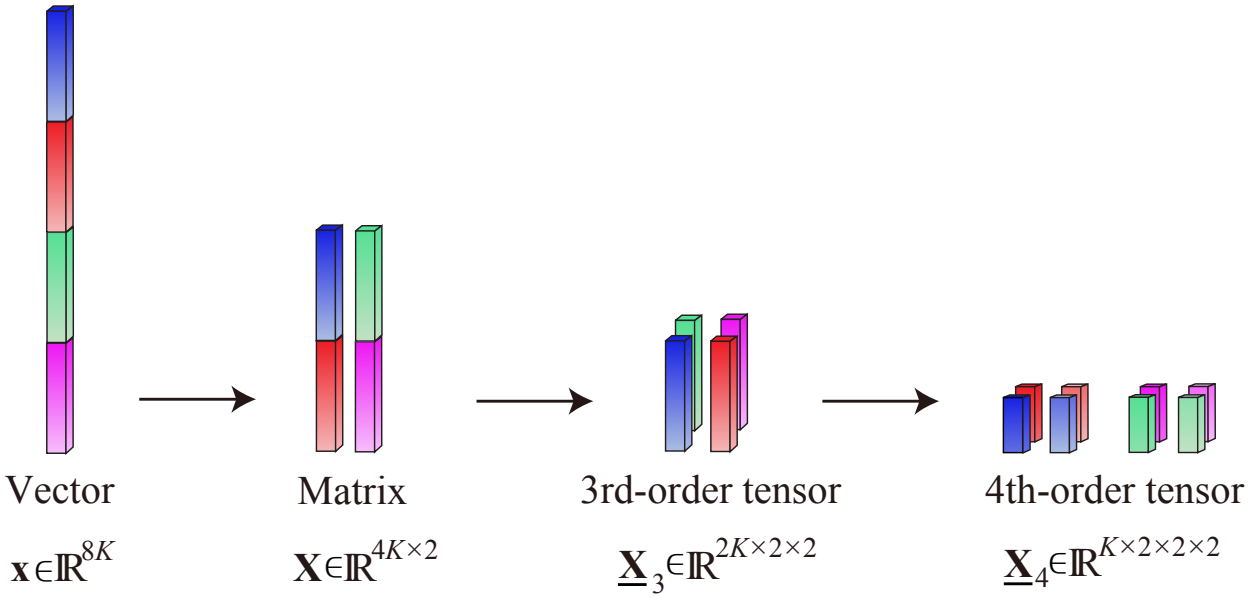
$$\begin{bmatrix} a & az & az^2 & az^3 & \cdots \end{bmatrix} \tag{1}$$

- 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 13)
- **Mathematical construction**. Through e.g. time x frequency x channel representation
- **Experimental design.** EEG data over I channels, J subjects, K trials (Slides 17-18)
- **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 40)

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

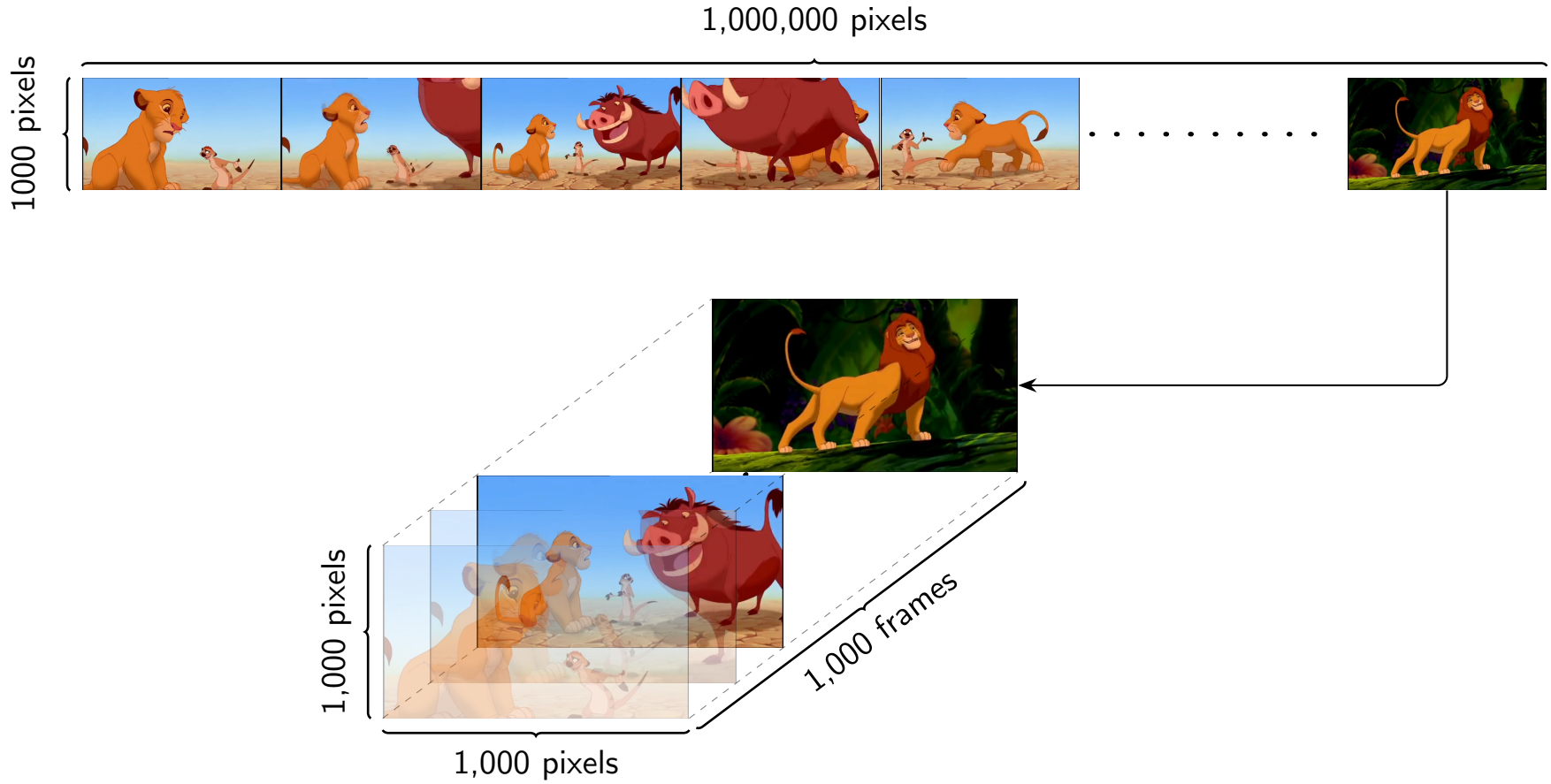
A video clip can be seen as a short & wide matrix $\mathbf{X} \in \mathbb{R}^{1,000 \times 1,000,000}$

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

- Significant difference in dimensions $\not\rightarrow$ 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

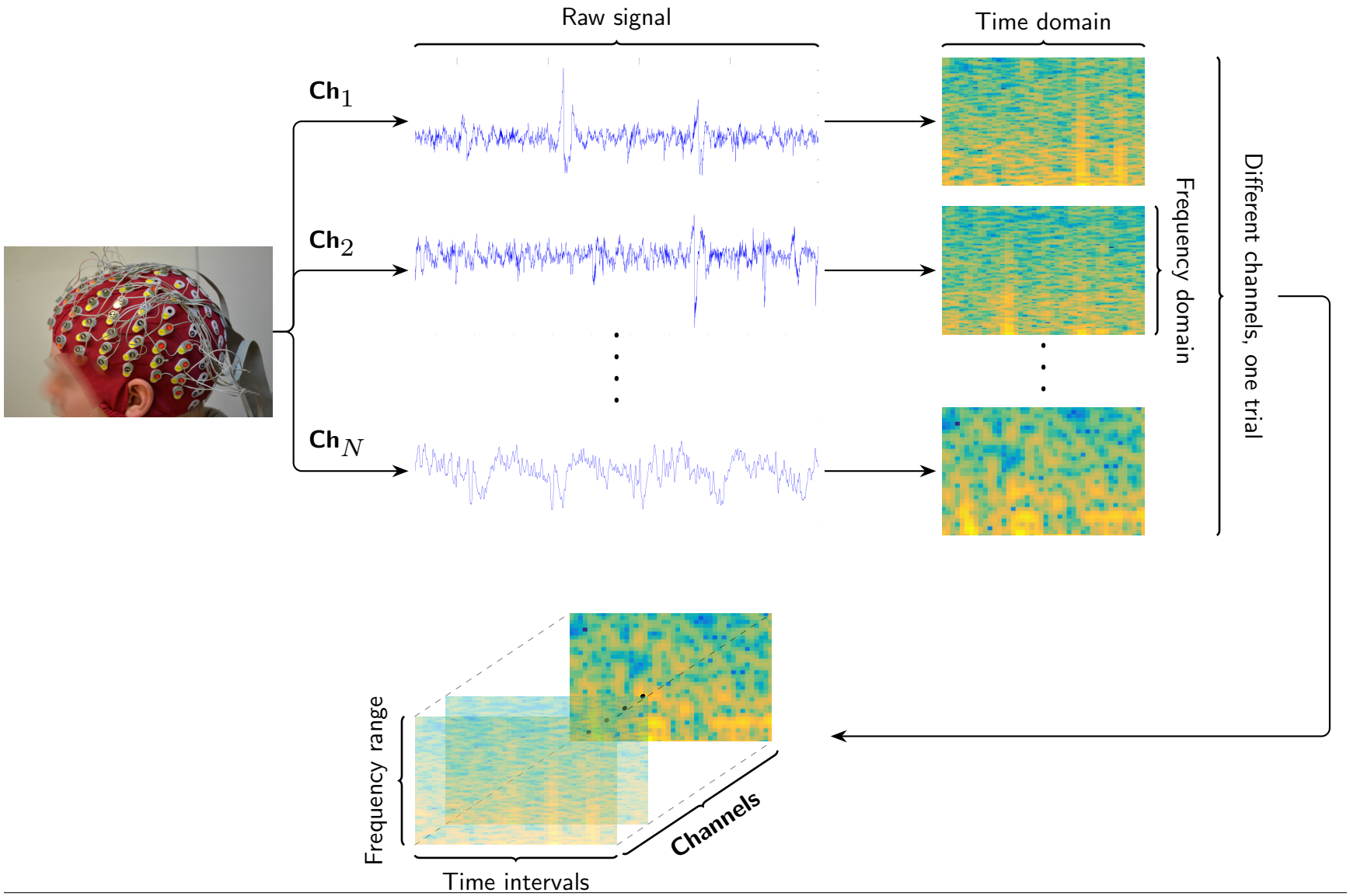
Example 1: Video clip ↬ tensor construction



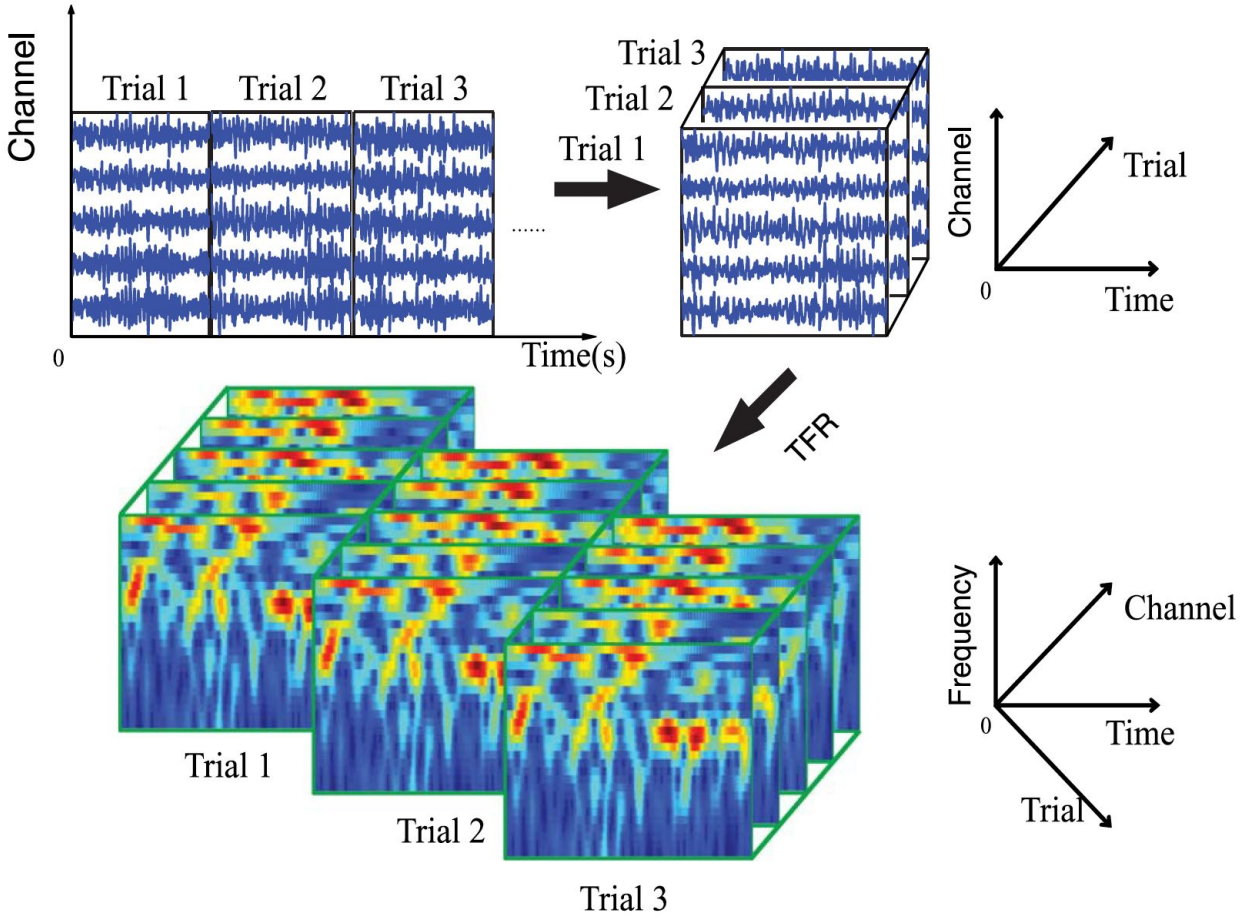
- A simple re-arrangement into a cube transforms the 1,000 × 1,000,000 matrix of frames into a 3-way tensor of size 1,000 × 1,000 × 1,000

Example 1a: Tensor construction from different channels

↬ channel × frequency × time



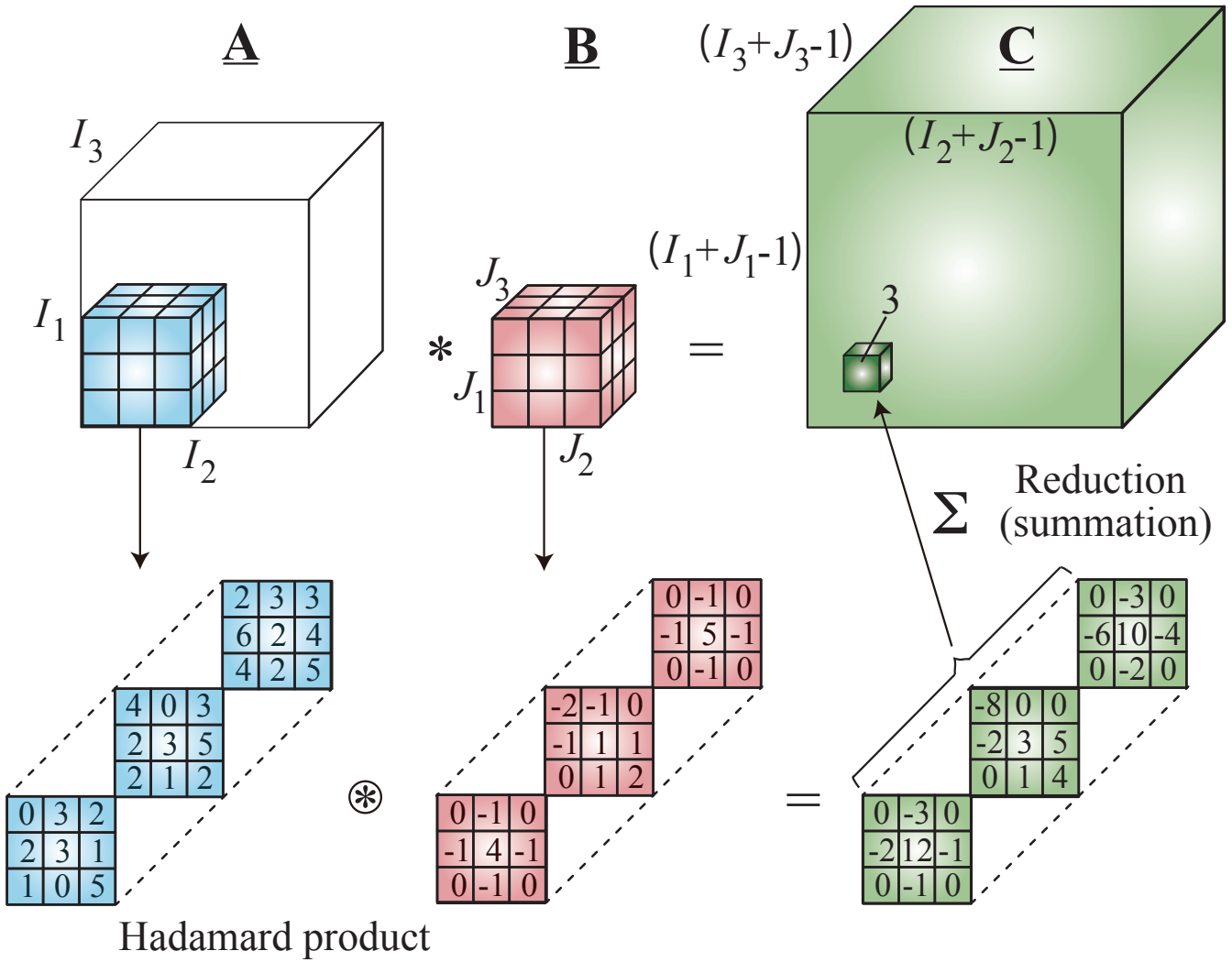
Example 1d: Putting it all together, construction of a 4D tensor with modes channel × trial × frequency × time



- 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

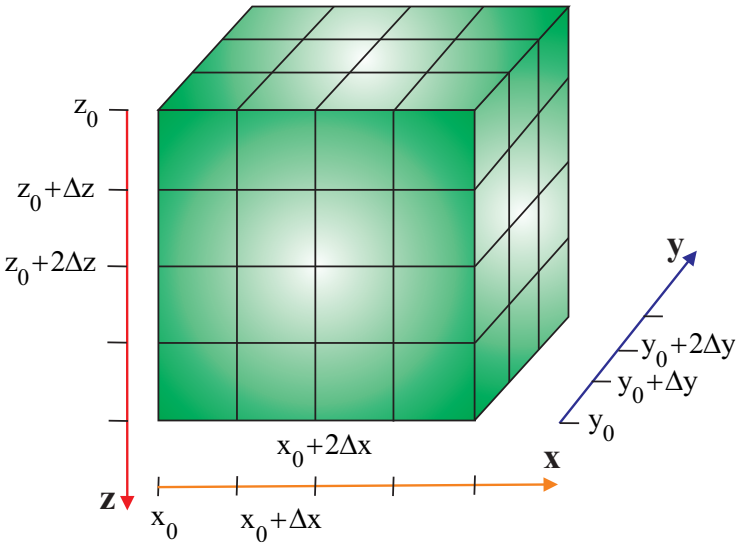
Example 2: Connection with 'flat' DSP, 3D convolution

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 3: Scientific computing

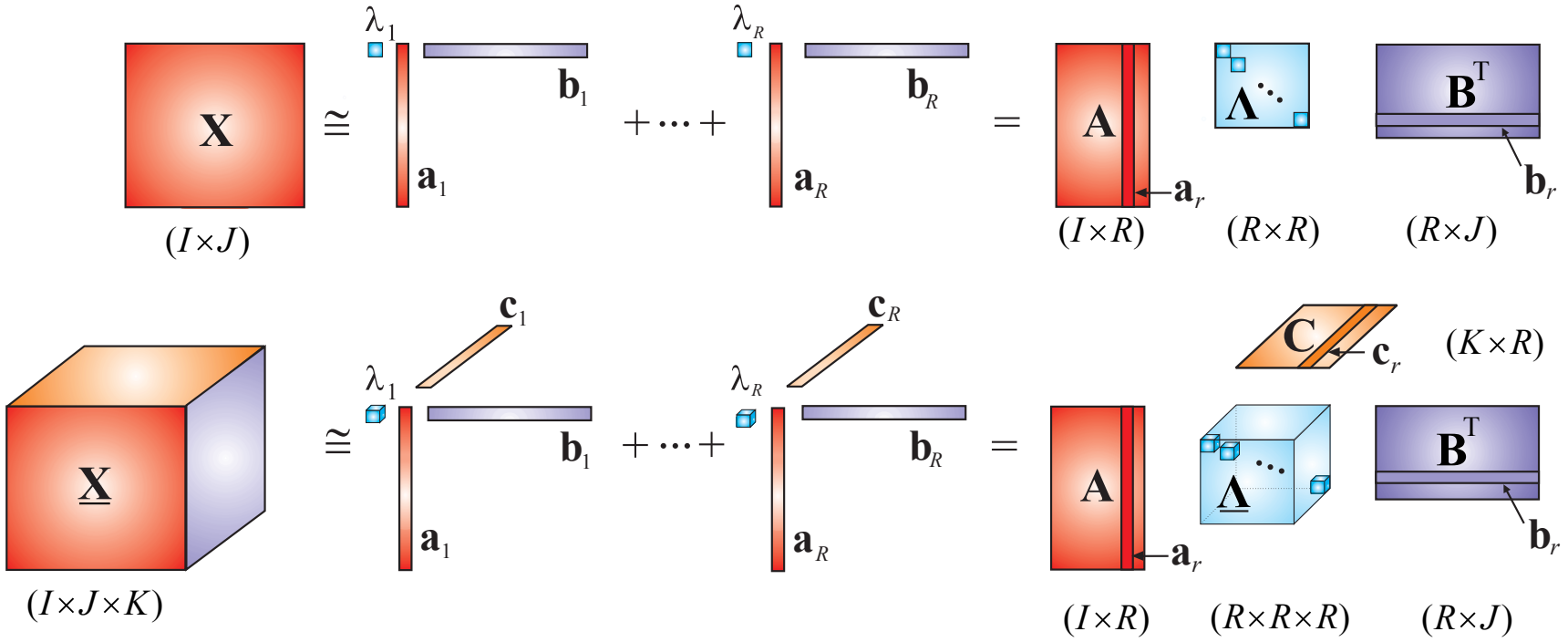
For computational purposes we often need to sample a multidimensional function on a grid (e.g. brain scans)

- 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)

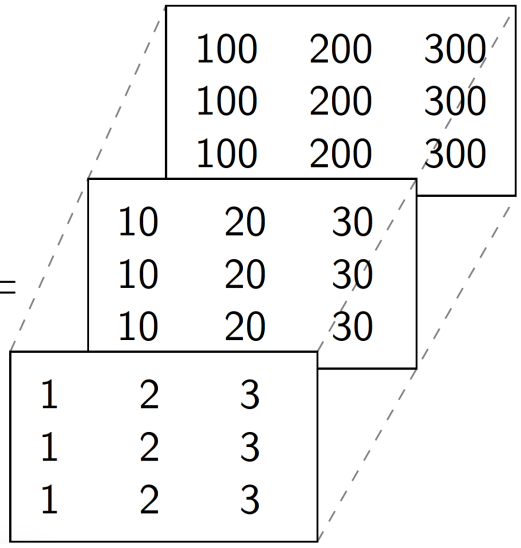
Example 4: The outer product in three dimensions

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

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

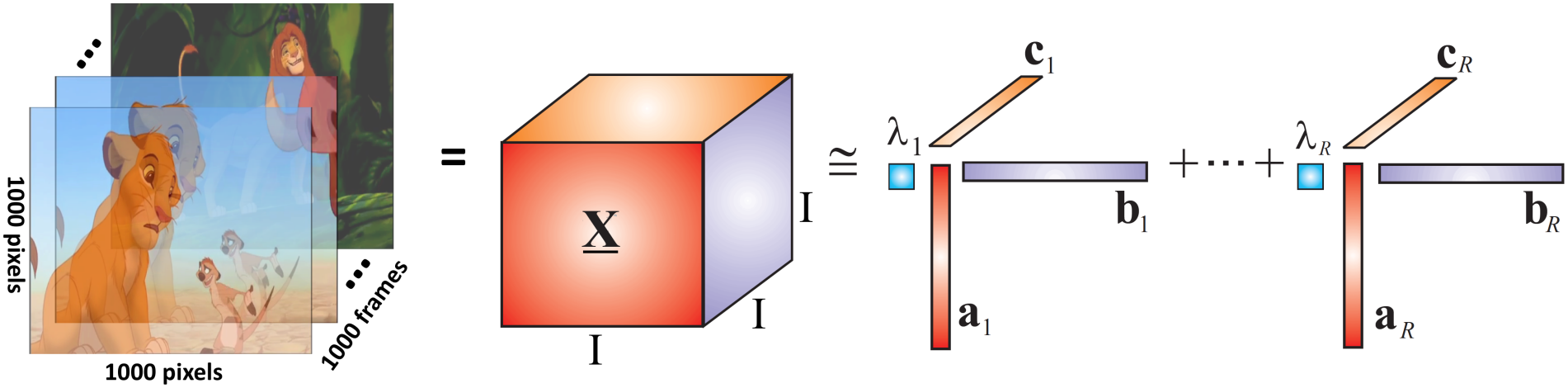
$$\mathbf{a} \circ \mathbf{b} \circ \mathbf{c} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \circ \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \circ \begin{bmatrix} 1 \\ 10 \\ 100 \end{bmatrix}$$

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



Example 5: CPD applied to our video-clip example

Inherent compression within the CPD ↬ storage and computational advantages



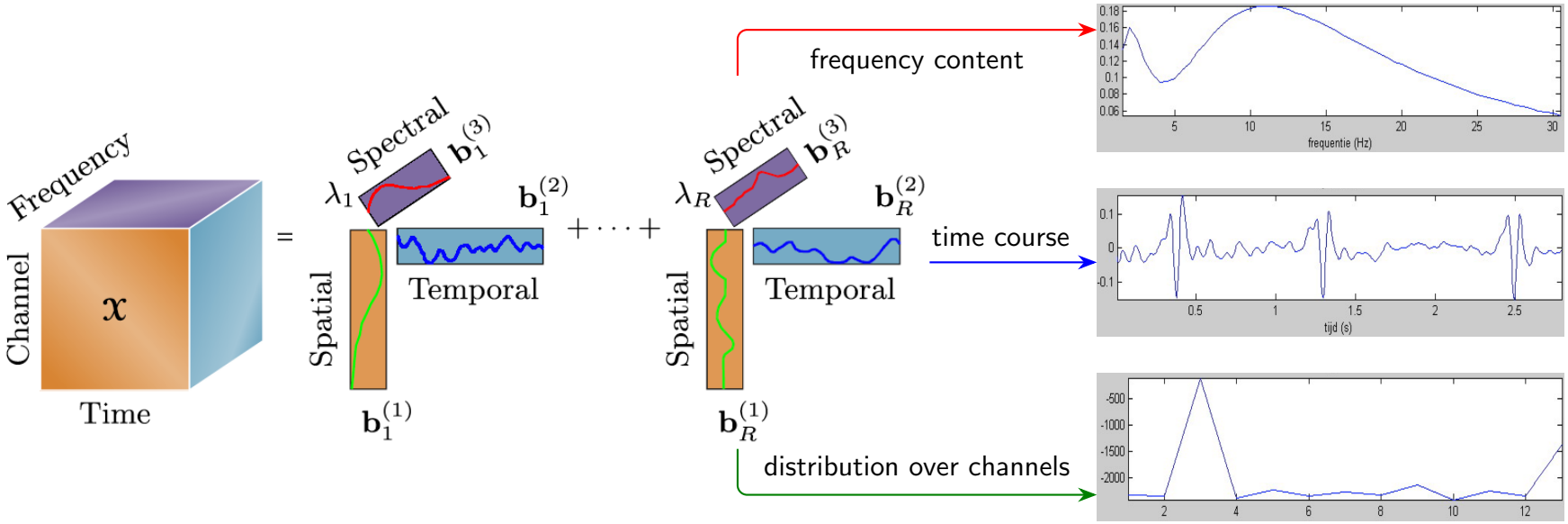
After tensorizing the video clip, tensor order $N = 3$, the dimension in every mode $I = 1000$, and the tensor rank is R. Typically $R \lll I$.

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

- **Raw data format** ↬ $I^N = 1000 \times 1000 \times 1000 = 10^9$ 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 $\rightsquigarrow 4 \times 10^5$ samples in CPD

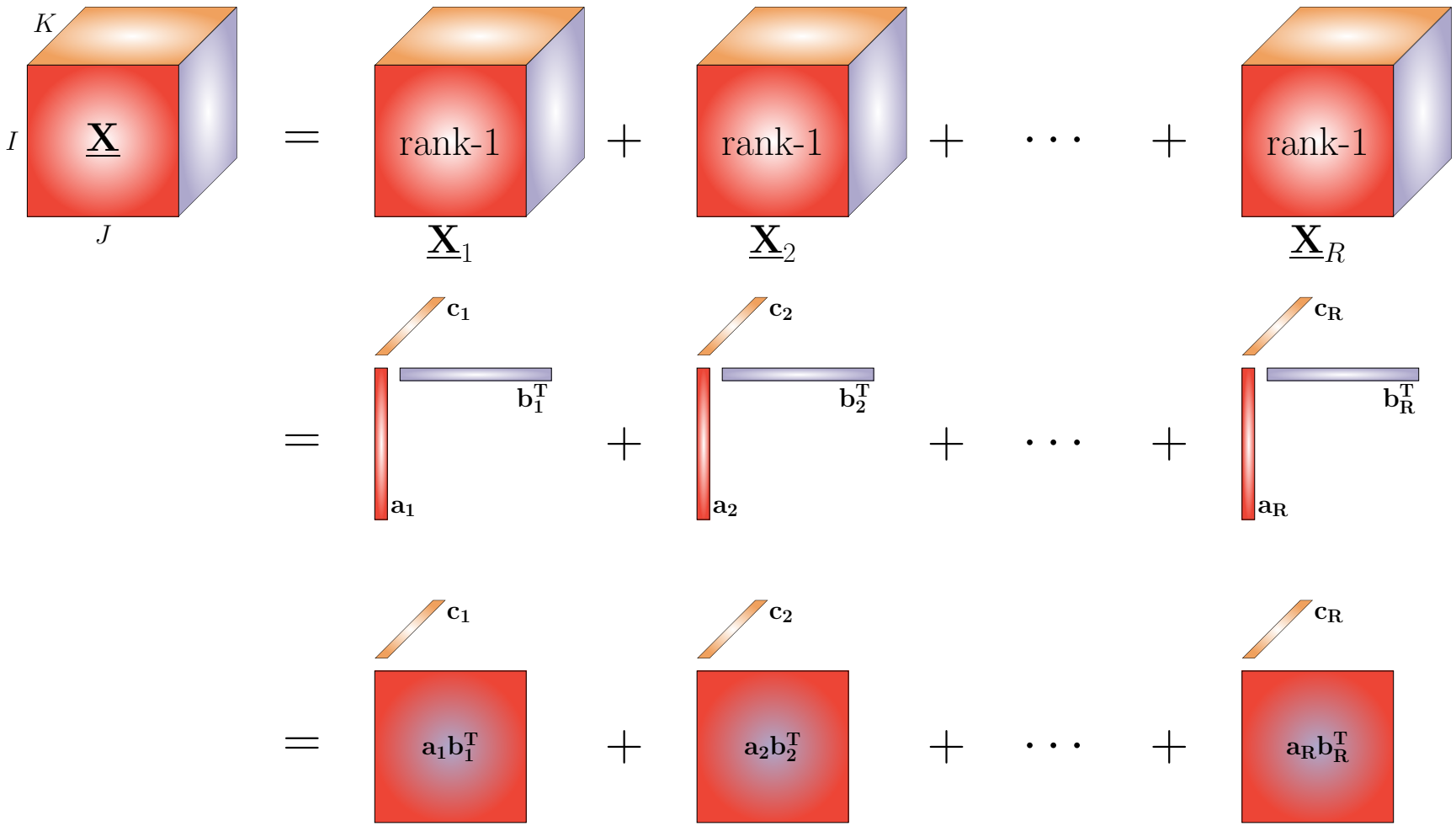
Intuition and physical meaning behind the CPD



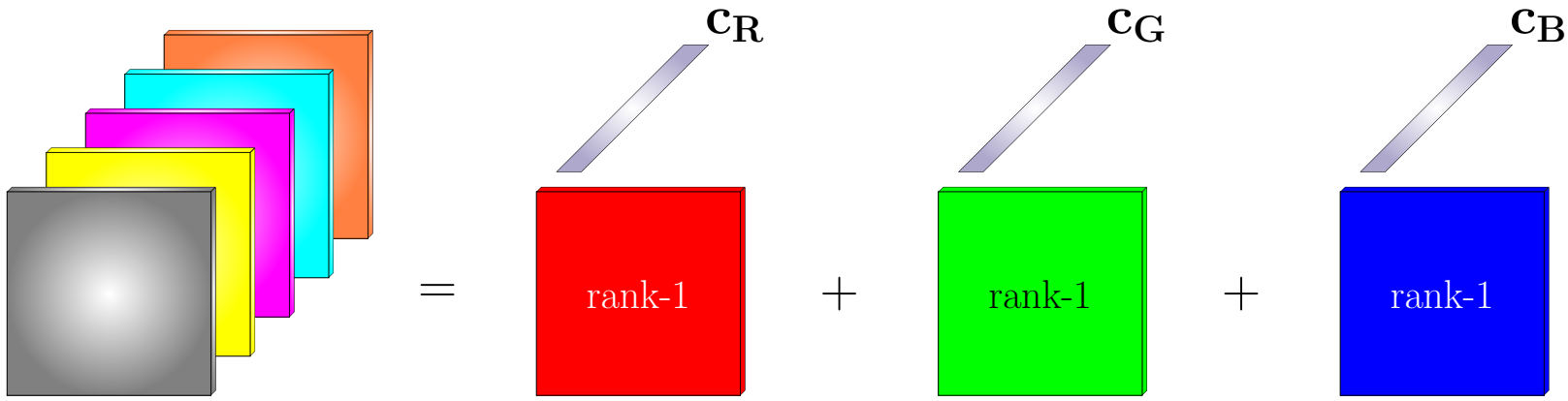
- Components $\mathbf{b}_i^{(1)}, \mathbf{b}_i^{(2)}, \mathbf{b}_i^{(3)}$ (factor 1) are associated with one another (linked)
- However, none of them is associated with any other set of such components (factors) for $i \neq j$, e.g. with $\mathbf{b}_R^{(1)}, \mathbf{b}_R^{(2)}, \mathbf{b}_R^{(3)}$
-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

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \lambda_r \cdot \mathbf{b}_r^{(1)} \circ \mathbf{b}_r^{(2)} \circ \mathbf{b}_r^{(3)} = [\![\underline{\mathbf{D}}; \mathbf{B}^{(1)}, \mathbf{B}^{(2)}, \mathbf{B}^{(3)}]\!] \tag{4}$$

From matrix rank to tensor rank



Example 6: Intuition behind the tensor rank

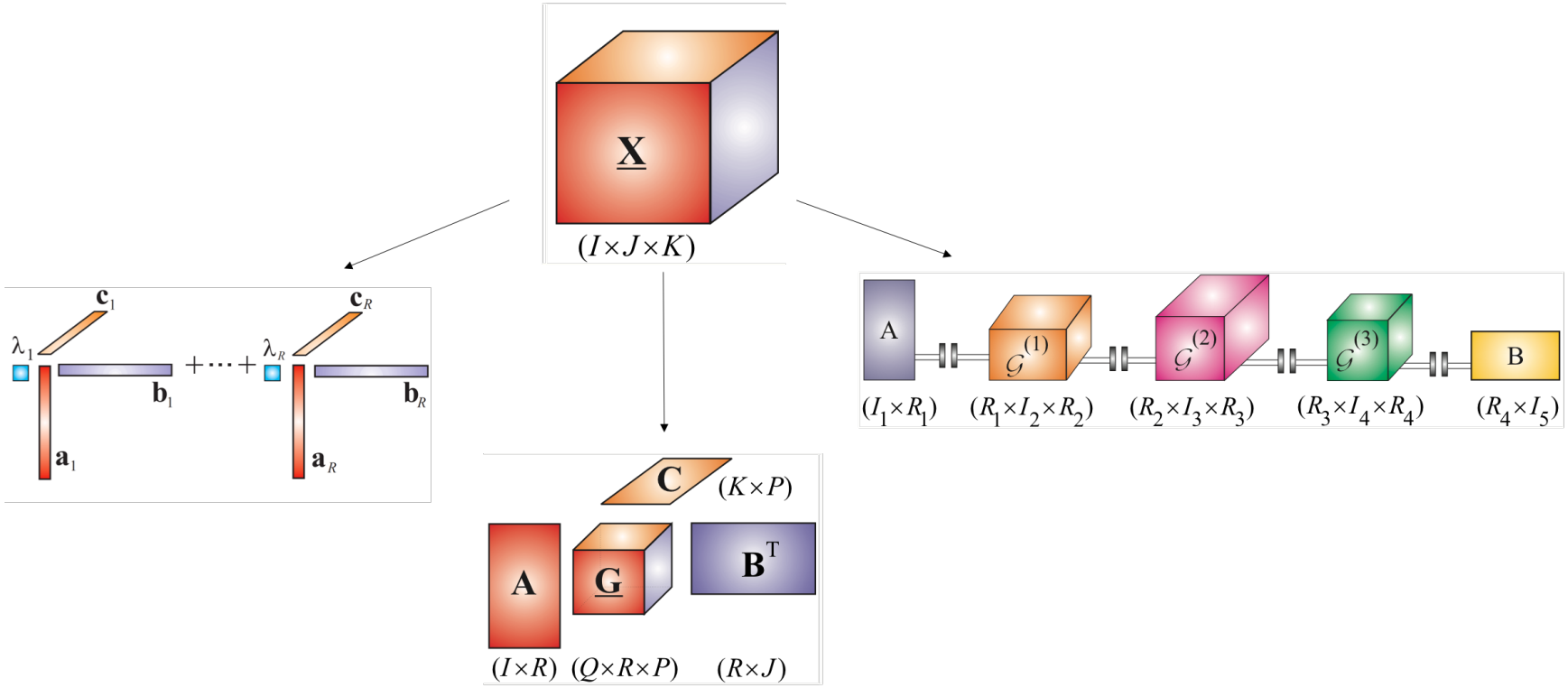


- All colors are just combination of three base colors: red, green and blue $\leadsto$ rank $= 3$
- Vectors $\mathbf{c}_R, \mathbf{c}_G, \mathbf{c}_B$ represent intensity, i.e. each value characterises how much of the base color there is in the corresponding slice

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

Tensor decompositions ↬ Blessing of dimensionality

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

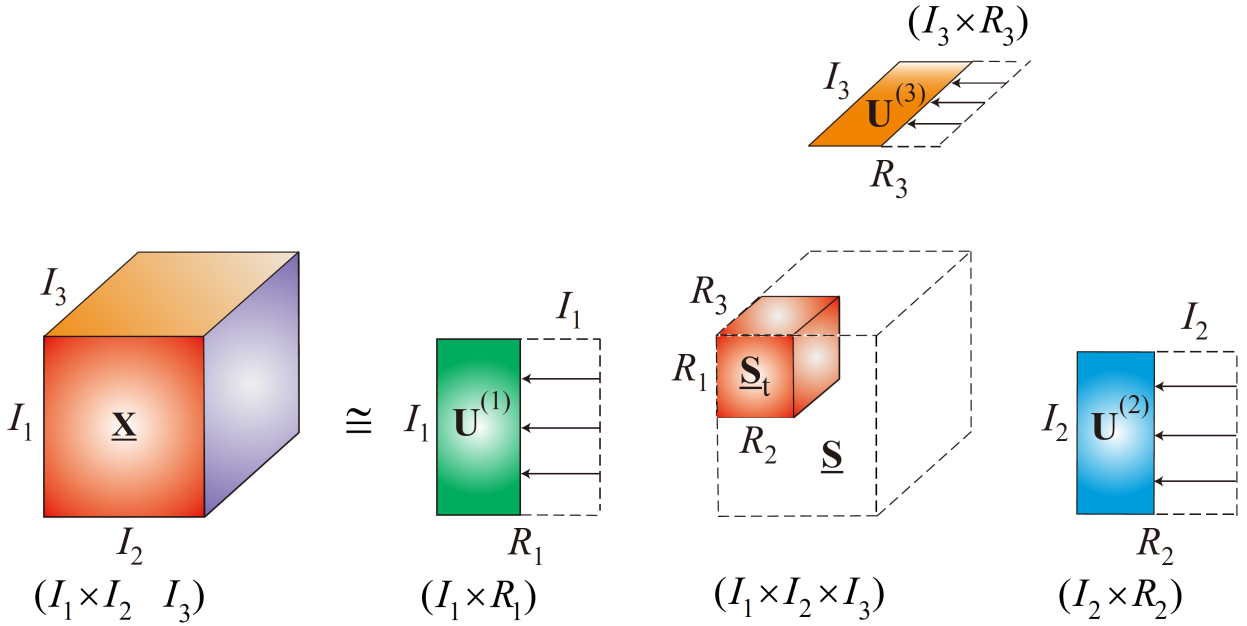


- Can represent tensors with fewer parameters
- Overcome storage issues
- Allow the application of algorithms which would otherwise be prohibitive, to the extremely high computational cost

Tucker Decomposition (TKD)

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

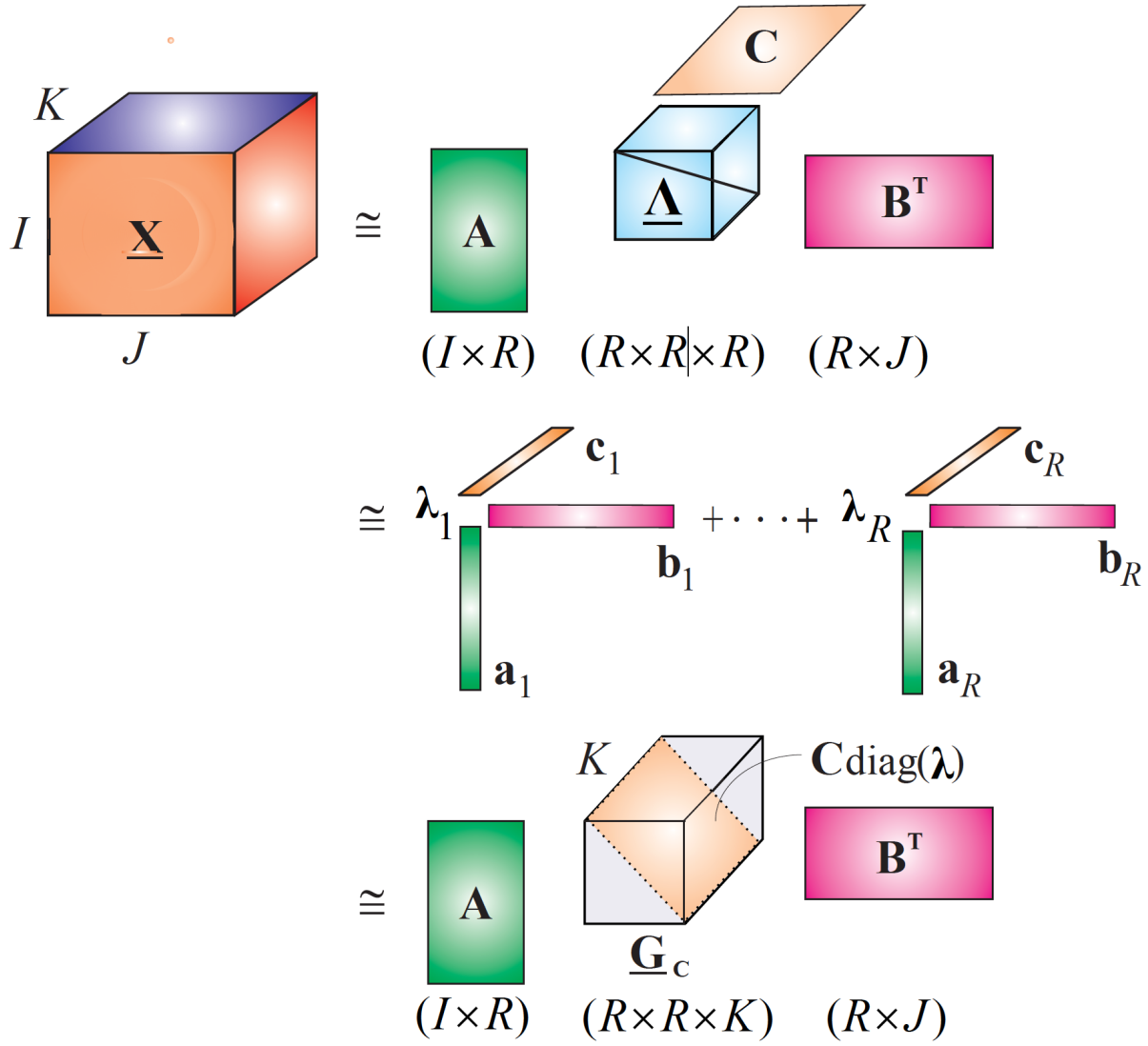
The TKD is not unique, but the subspaces defined by $\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)}$ are unique



- 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

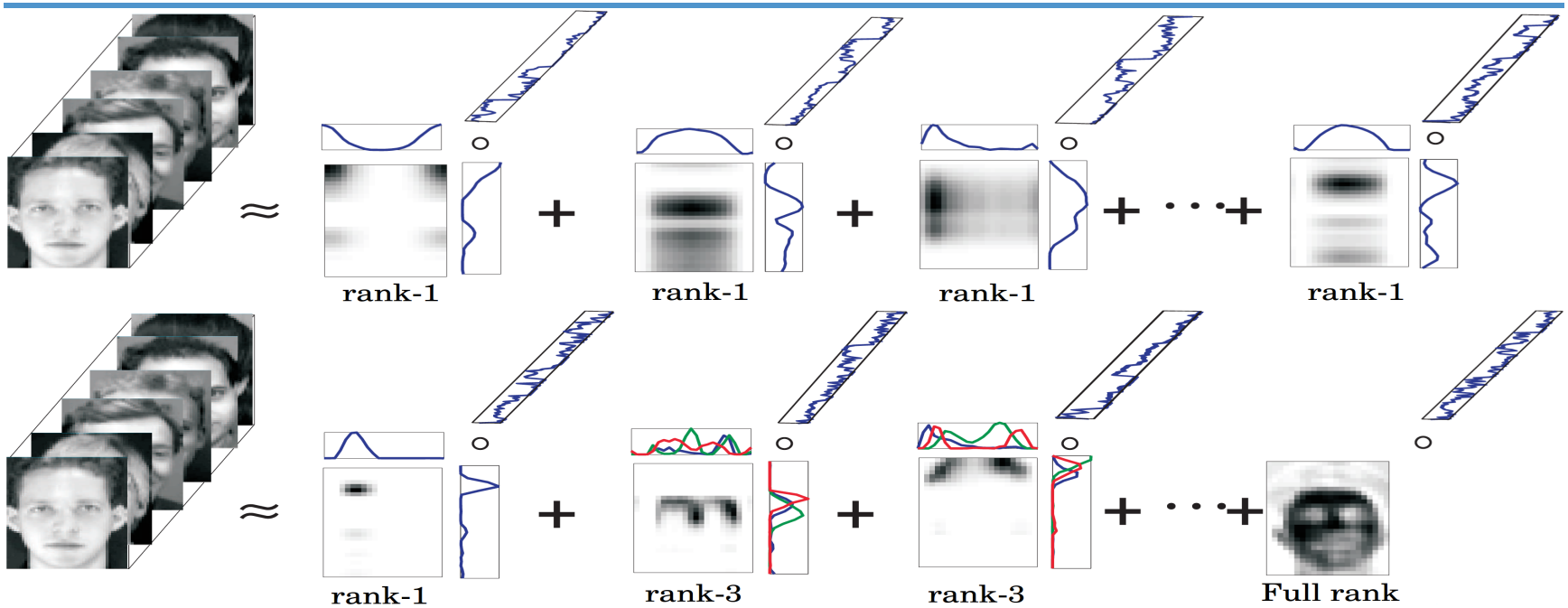
CPD = TKD with a diagonal core



Block Term Decomposition (BTD)

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

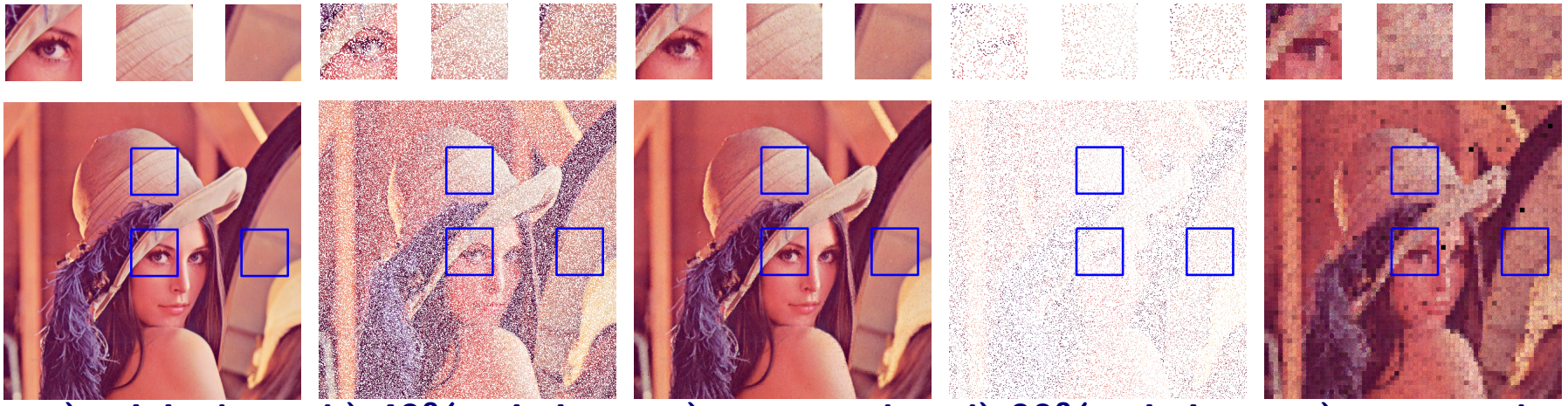
Top: CPD $\rightsquigarrow$ sum of rank-1 tensors **Bottom:** BTD $\rightsquigarrow$ generalization of CPD



- 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 7: Tensor completion (missing data recovery)

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



a) original b) 40% missing c) recovered d) 90% missing e) recovered

- 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 14), 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 40)

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

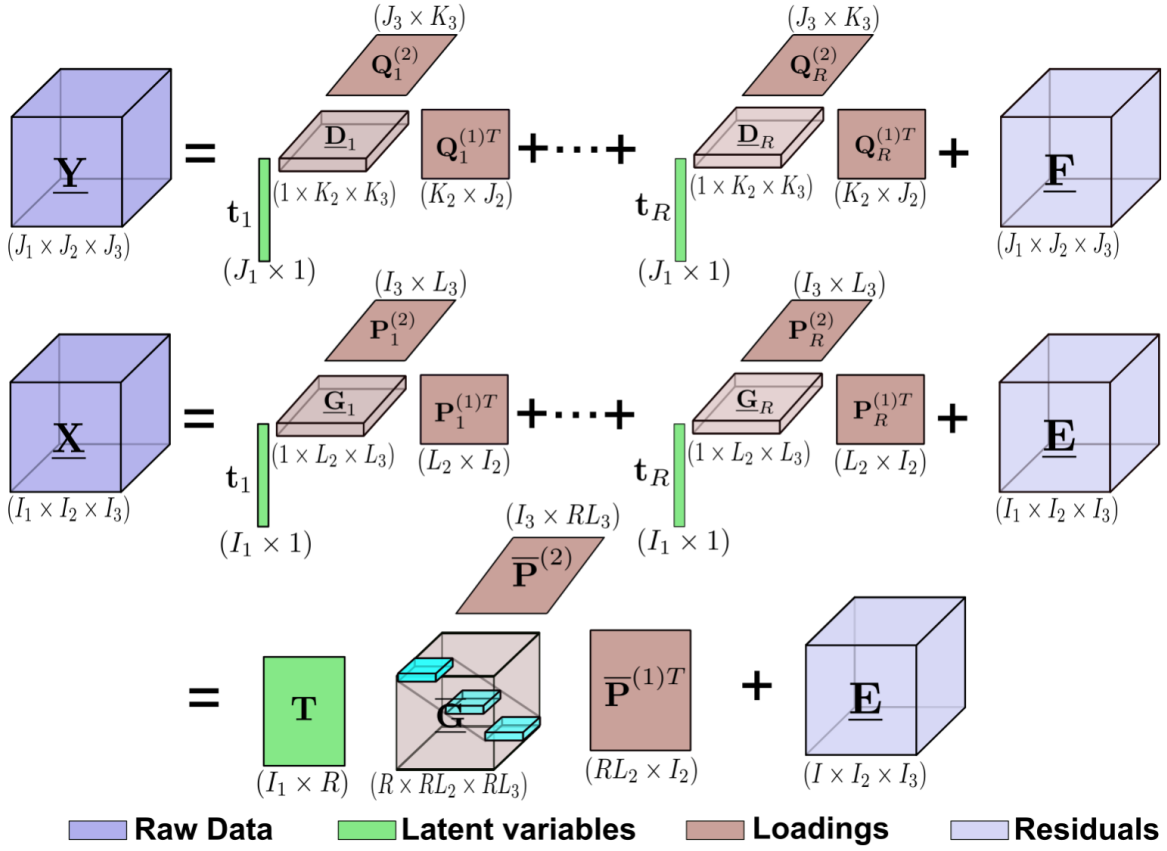
- Regression refers to the modelling of one or more dependent variables (outputs, responses), $\mathbf{Y}$, by a set of independent variables (regressors, predictors), $\mathbf{X}$
- Concept behind PLS ☞ underlying structure is governed by latent variables shared between the $\mathbf{X}$ and $\mathbf{Y}$
- 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)

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

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

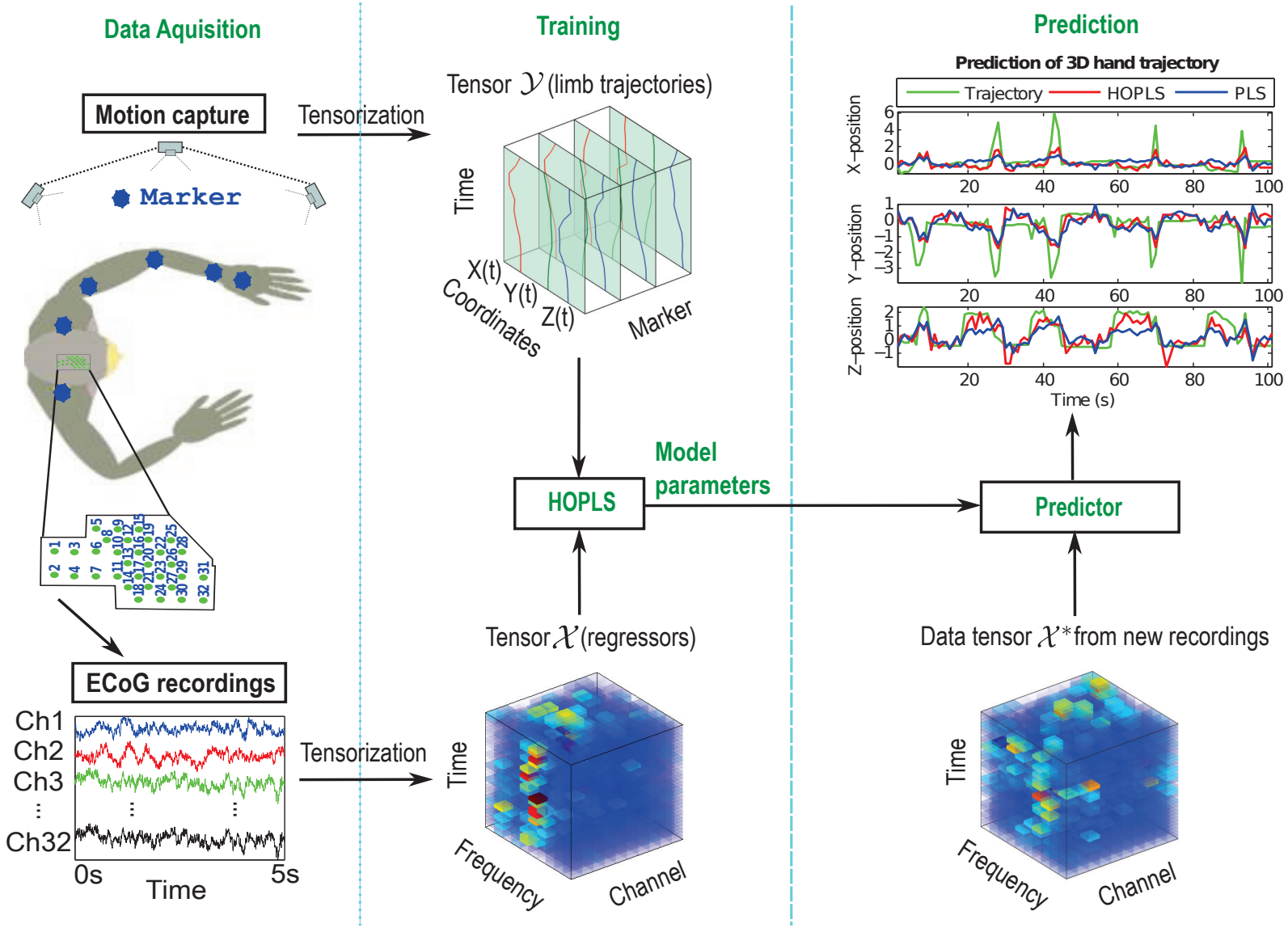
Tensor-valued PLS
The Higher-Order Partial Least Squares (HOPLS)

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



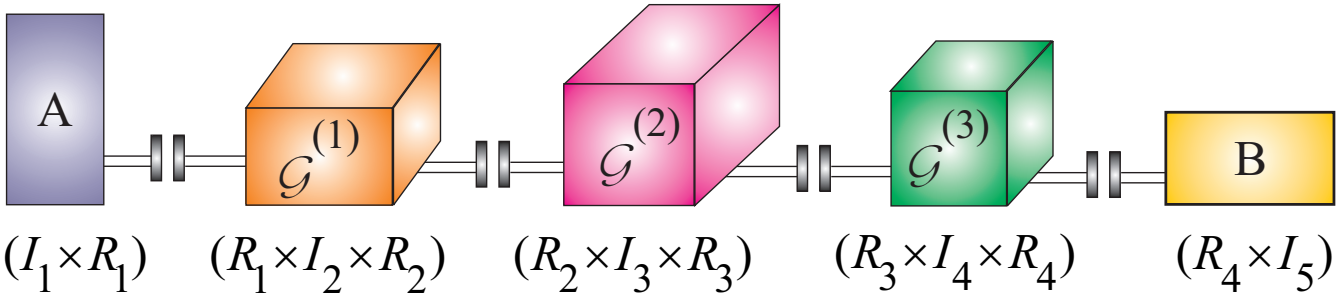
Example 8: Prediction of arm movement from brain activity

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

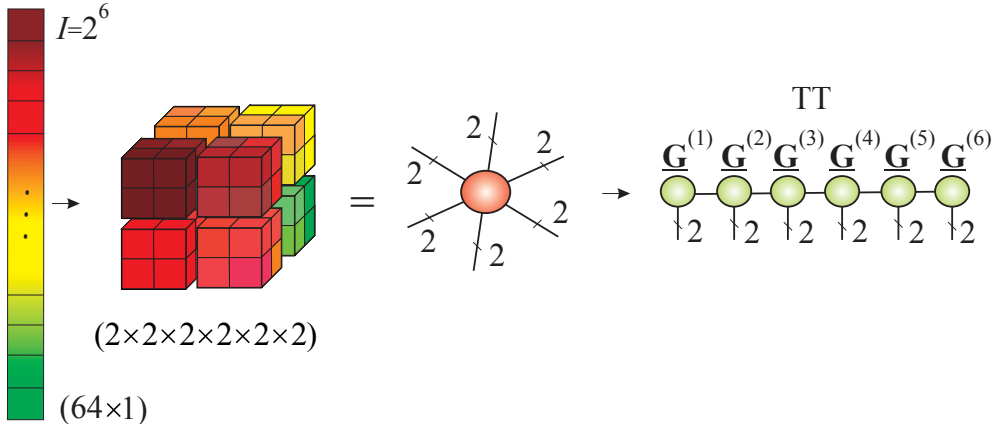


Advanced concepts: Tensor train (TT) decomposition

Curse of dimensionality can be eliminated through tensor network representations

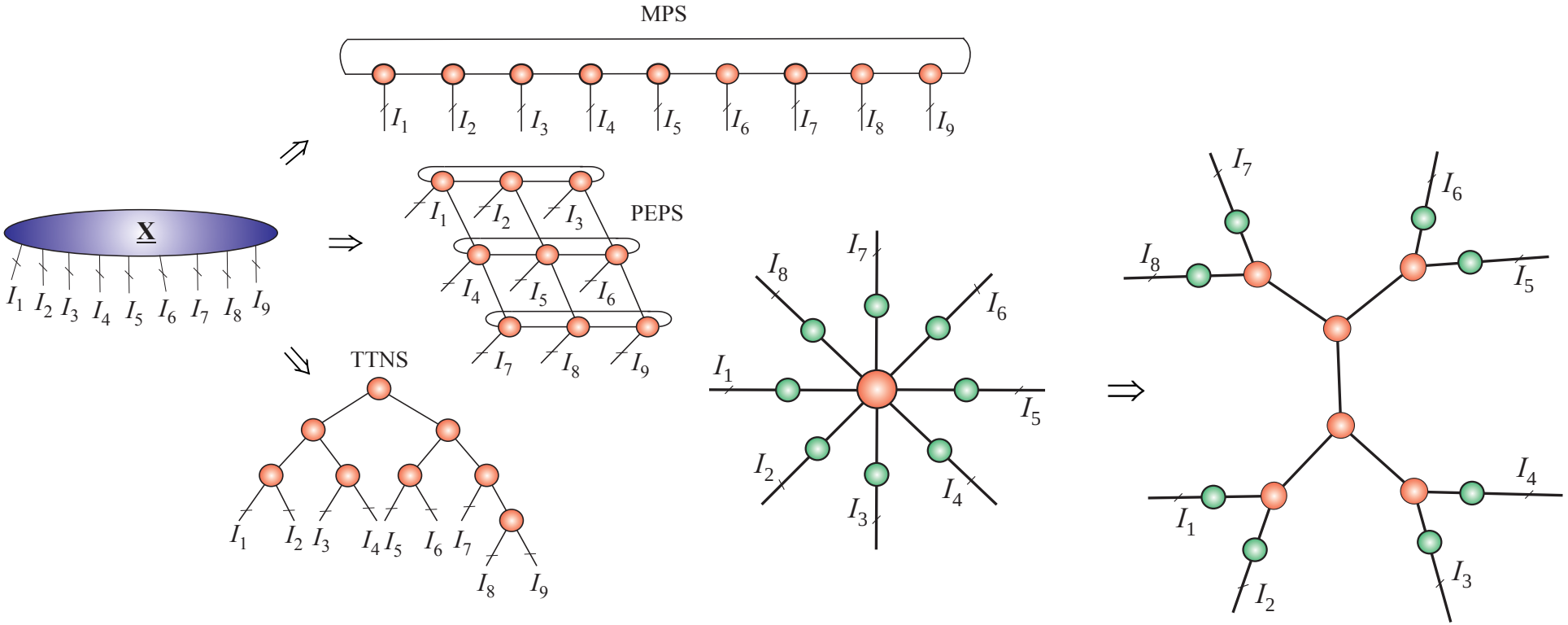


- More degrees of freedom $\rightsquigarrow$ more latent dependencies need to be preserved
- This inevitably leads to *curse of dimensionality (CoD)* (see Slide 20) $\not\hookrightarrow$ the number of elements grows exponentially with the the tensor order (number of dimensions)
- TT decomposition represents 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)

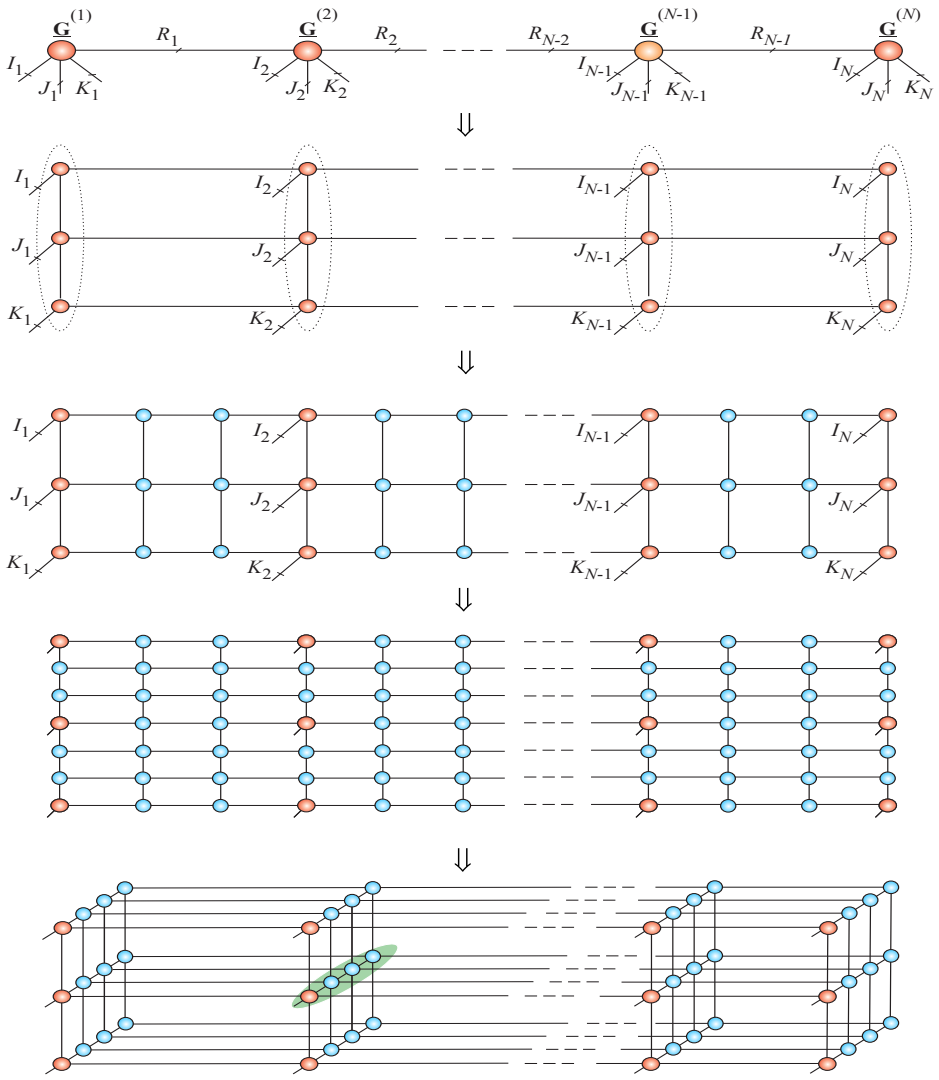


- Tensor network architectures can be with or without loops ↬ the Matrix Product State (MPS), Tree Tensor Network State (TTNS), Projected Entangled-Pair States (PEPS), Hierarchical Tucker (HT)
- TNs decompose a very high-order tensor into sparsely (weakly) connected low-order and small-size core tensors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

More complex tensor networks (TNs)

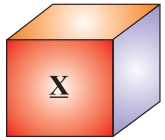
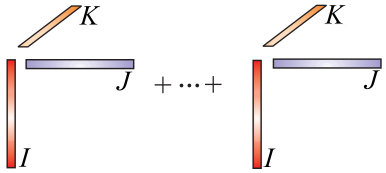
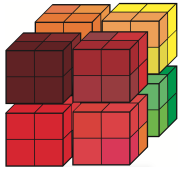
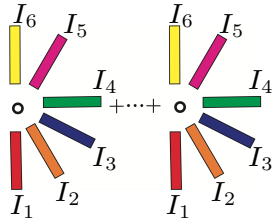
Representing a high order tensor as a set of matrices and lower order tensors

- 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 $\not\hookrightarrow$ the Matrix Product State (MPS), Tree Tensor Network State (TTNS), Projected Entangled-Pair States(PEPS), Hierarchical Tucker (HT)



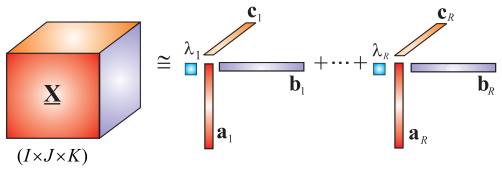
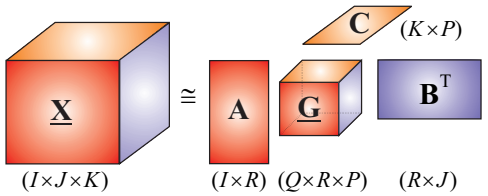
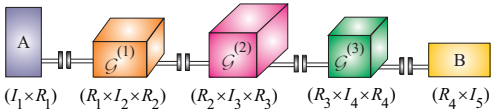
Super-compression inherent to TNs

Exponential complexity for the raw data format $\rightsquigarrow$ linear complexity for TDs

Data format	length(mode$_n$)=10	length(mode$_n$)=10^m	General case	Number of elements in a data format
 $(I \times J \times K)$	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}	$\prod_{n=1}^{6} I_n$	
	$R \cdot 6 \cdot 10$	$R \cdot 6 \cdot 10^m$	$R \sum_{n=1}^{6} I_n$	

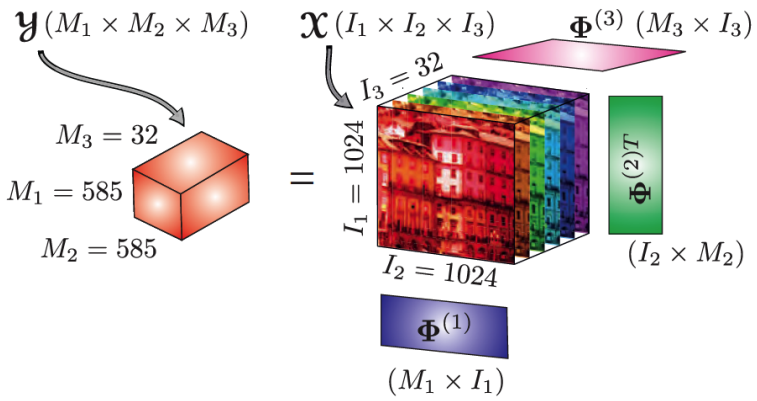
- R is the rank of a tensor $\underline{\mathbf{X}}$ $\looparrowright$ CPD is a sum of R rank-1 terms. On practice $R \ll I_n$
- For an N^{th}-order tensor all I^N elements are efficiently represented through the CPD as a linear (instead of exponential) function of number of elements in each mode

Comparison of multidimensional decompositions

CPD	Tucker	Tensor Train
		
storage complexity		
$\mathcal{O}(NIR)$	$\mathcal{O}(NIR + R^N)$	Depends on a choosen type
inherent structure		
Represented through rank-1 terms	Represented through core tensors and factor matrices	Represented through tensor contractions
uniqueness conditions		
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

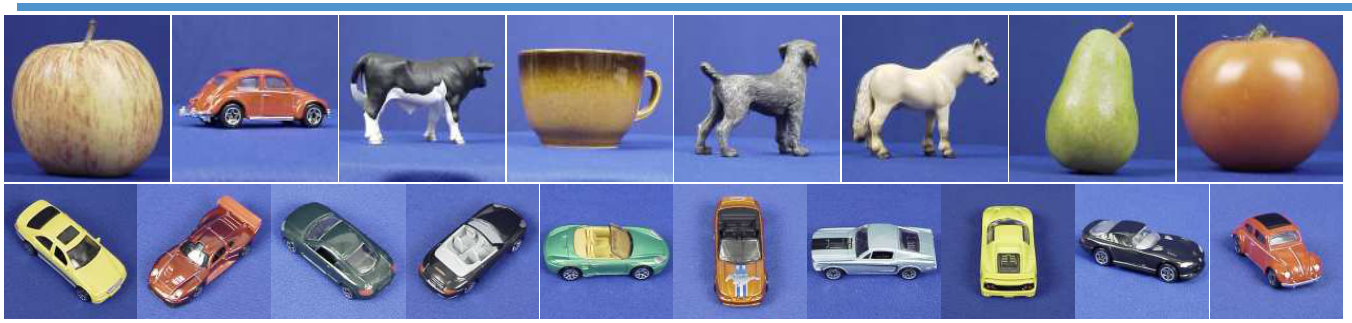
Original hyperspectral image - RGB display

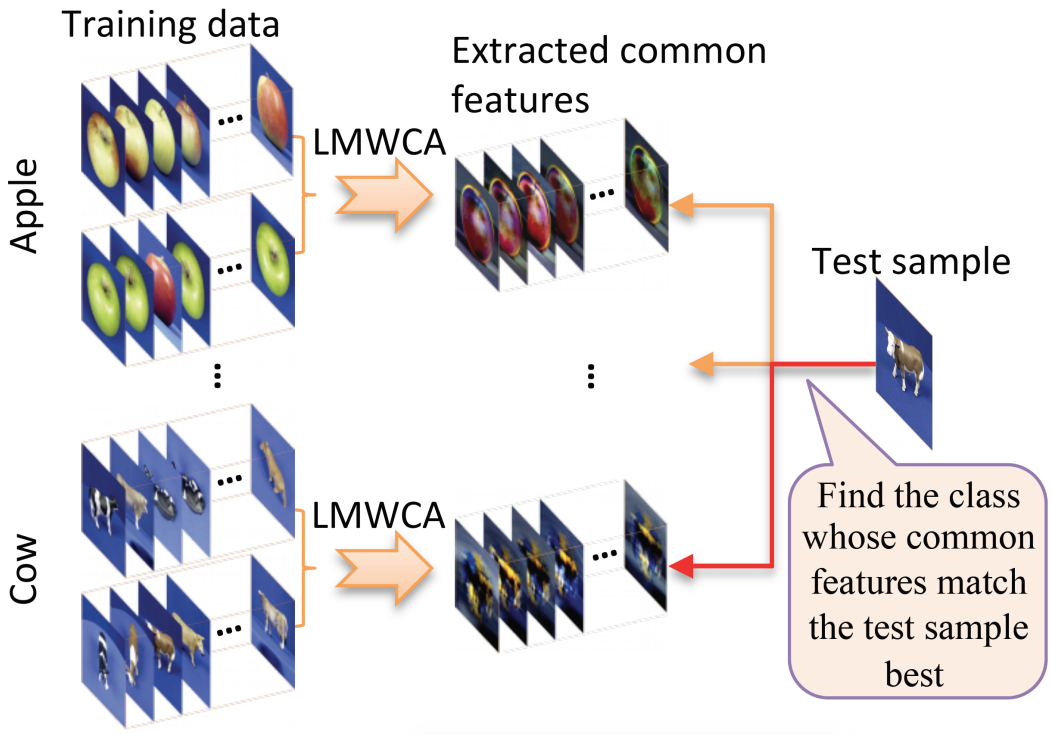
(1024 x 1024 x 32) (256 x 256 x 32)

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

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

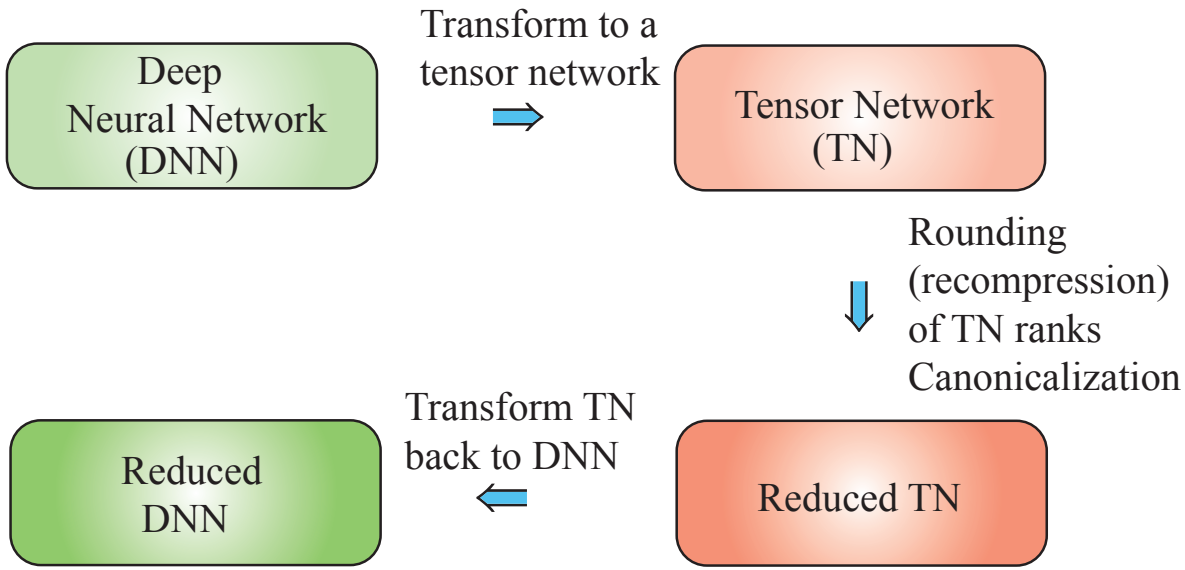
Example 9: Linked Multiway Component Analysis (LMWCA) for classification applications





- 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 $\leadsto$ better suited for classification

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



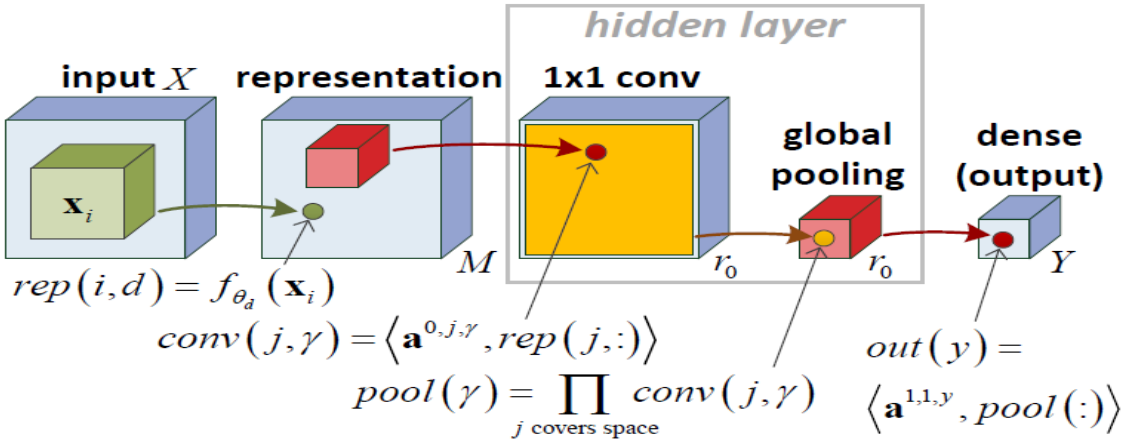
Depth efficiency ↬ DNNs can implement with polynomial size computations that would require super-polynomial size for shallow NNs.

☞ 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?

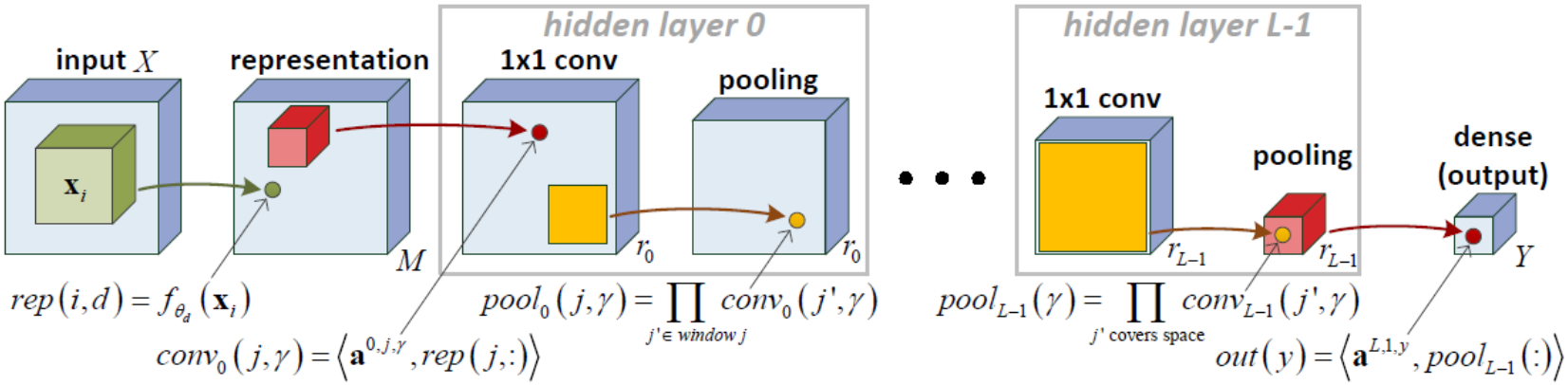
Opening the black box of Neural Networks

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, ...

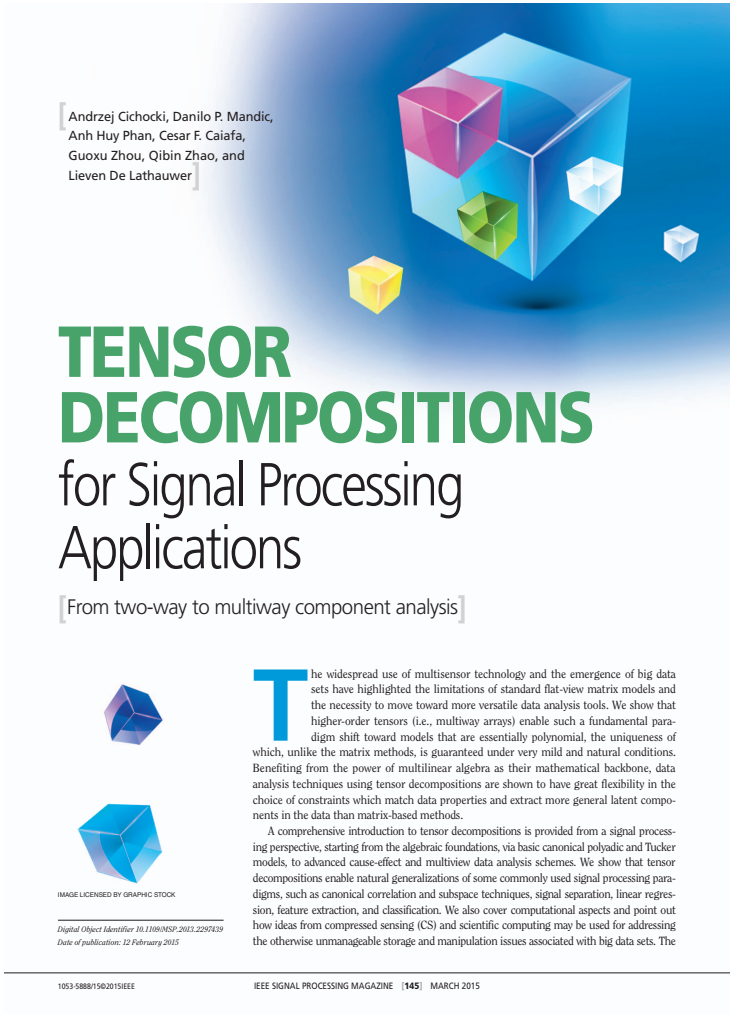
Literature

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

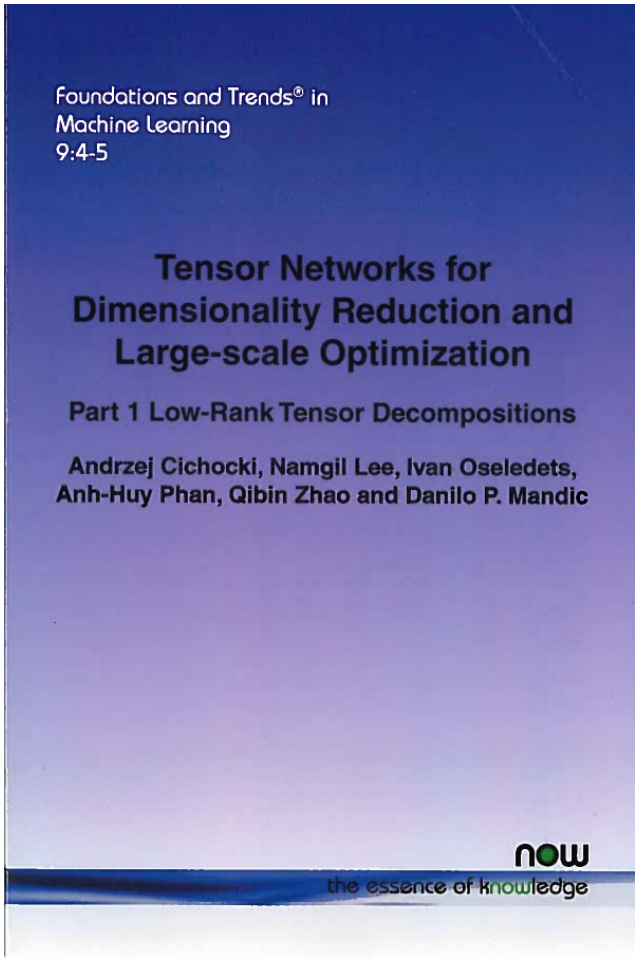
Check out our two-part monograph on Tensor Networks (Now Publishers, 2016, 2017)

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



IEEE SPM, March 2015

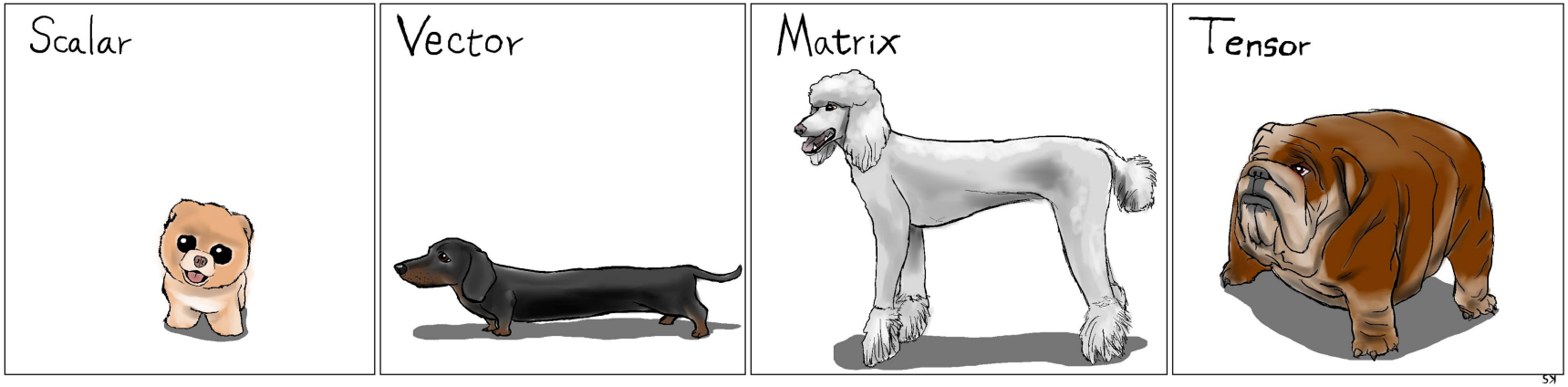
A. Cichocki, D. Mandic, *et al.*



Foundations and Trends in Machine Learning, Parts 1 & 2

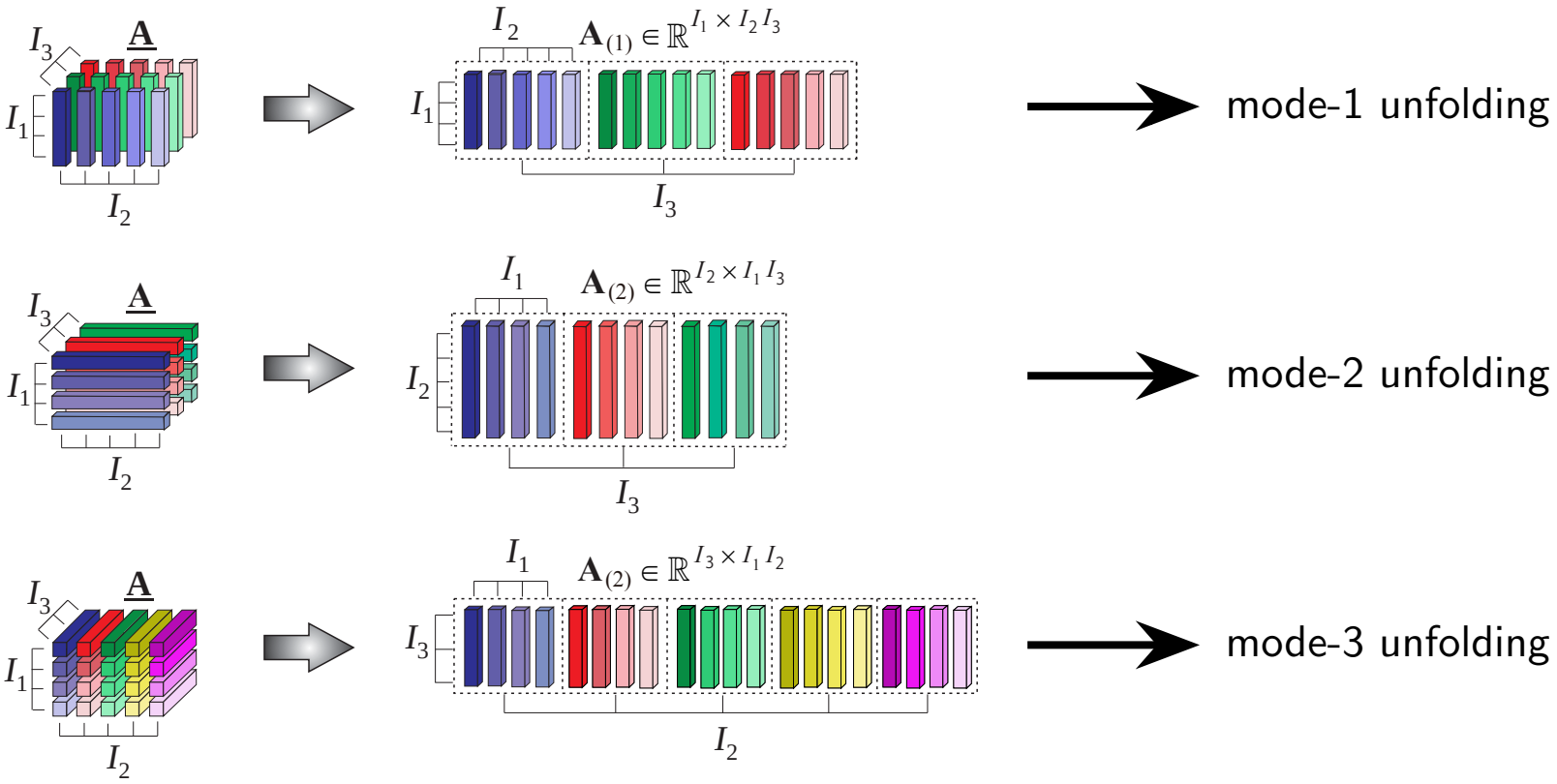
Tensors: Final Note

Thank you for your attention.
Any questions?



Unfolding of a tensor in different modes

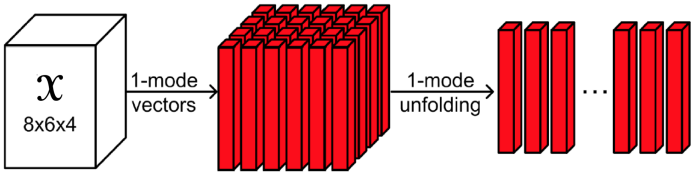
Converts a higher-order tensor into a smaller tensor, matrix, or vector



- 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

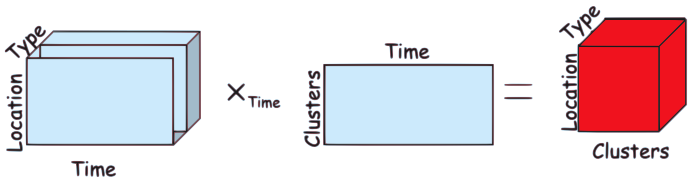
Mode-n unfolding



- 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:

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

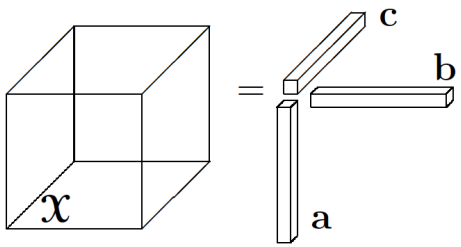
Mode-n product



- The mode-n product:

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

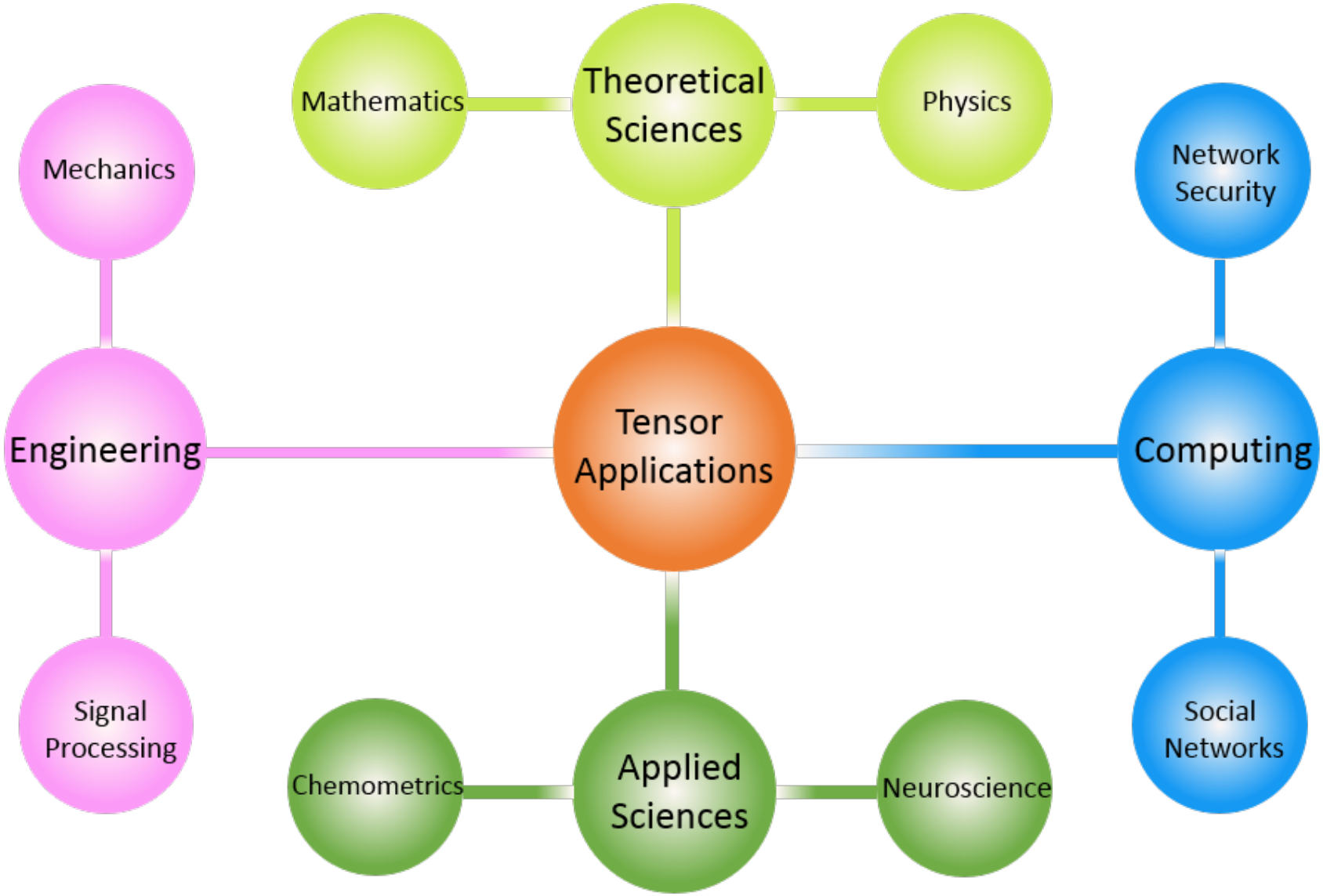
Outeproduct



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

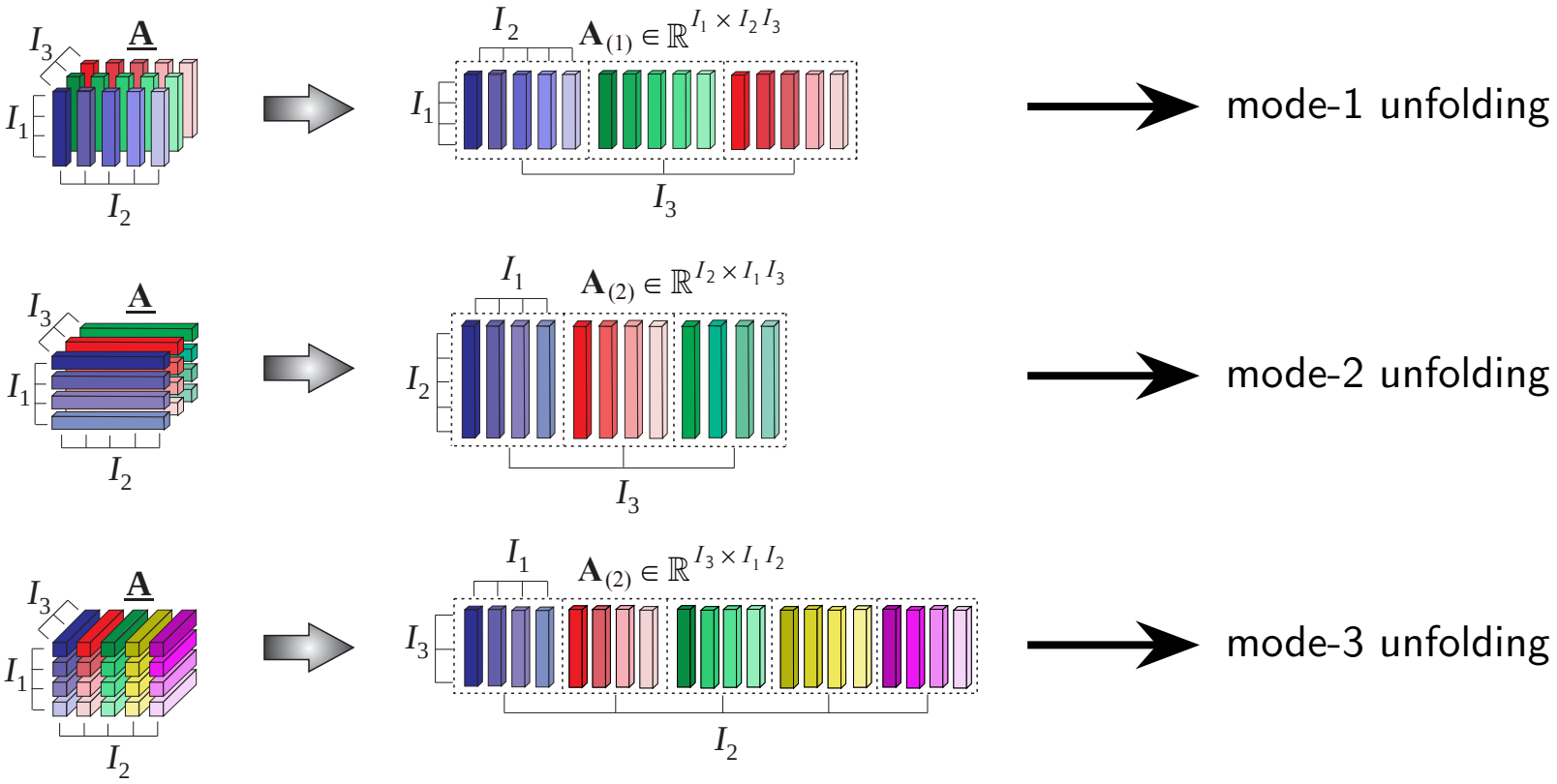
$$\mathbf{a}_1 \circ \mathbf{a}_2 \circ \cdots \circ \mathbf{a}_N = \underline{\mathbf{X}} \in \mathbb{R}^{I_1 \times \cdots \times I_N}$$

Tensors ↬ 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

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

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

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

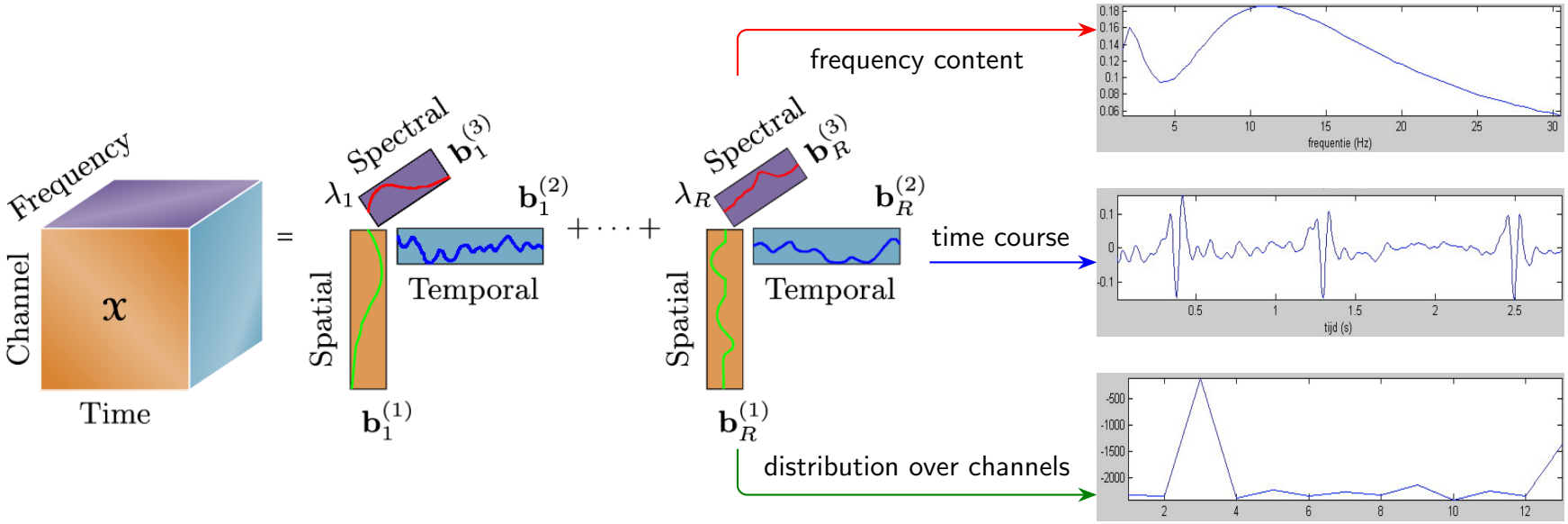
$$\mathbf{z}_{I:L} = \mathbf{Y}^T\mathbf{x} = \begin{bmatrix} y(I) & y(I-1) & y(I-2) & \cdots & y(1) \\ y(I+1) & y(I) & y(I-1) & \cdots & y(2) \\ y(I+2) & y(I+1) & y(I) & \cdots & y(3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y(L) & y(L-1) & y(L-2) & \cdots & y(J) \end{bmatrix} \begin{bmatrix} x(1) \\ x(2) \\ x(3) \\ \vdots \\ x(I) \end{bmatrix} \tag{6}$$

- 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

$$\mathbf{z} = \mathbf{x}_1 * \mathbf{x}_2 * \mathbf{y} \tag{7}$$

- First, a Toeplitz matrix $\mathbf{Y}$ is obtained from $\mathbf{x}_1 * \mathbf{x}_2$ as shown in Eq. (6)
- 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



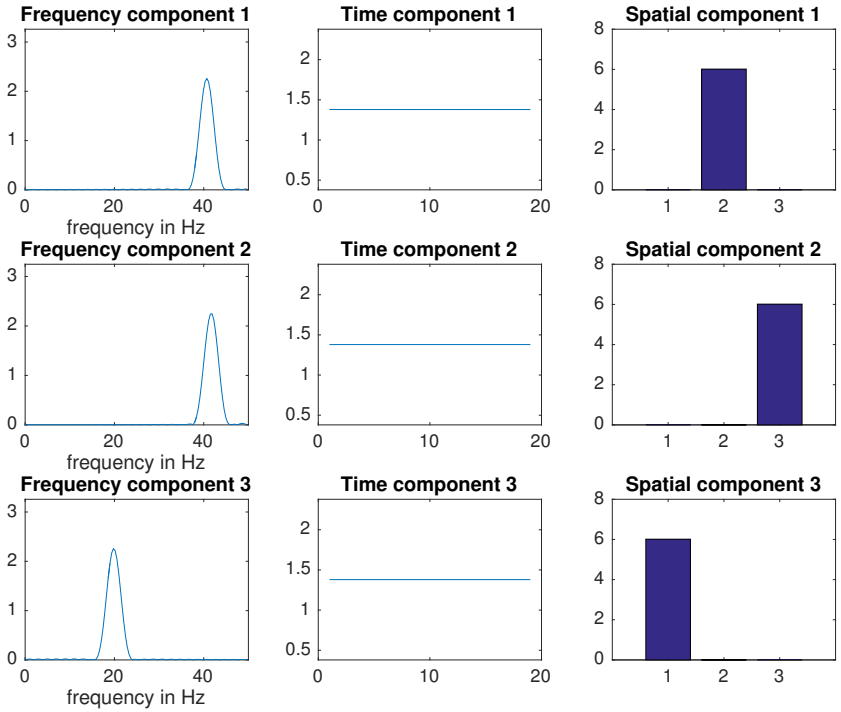
- Components $\mathbf{b}_i^{(1)}, \mathbf{b}_i^{(2)}, \mathbf{b}_i^{(3)}$ (factor 1) are associated with one another (linked)
- However, none of them is associated with any other set of such components (factors) for $i \neq j$, e.g. with $\mathbf{b}_R^{(1)}, \mathbf{b}_R^{(2)}, \mathbf{b}_R^{(3)}$
-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

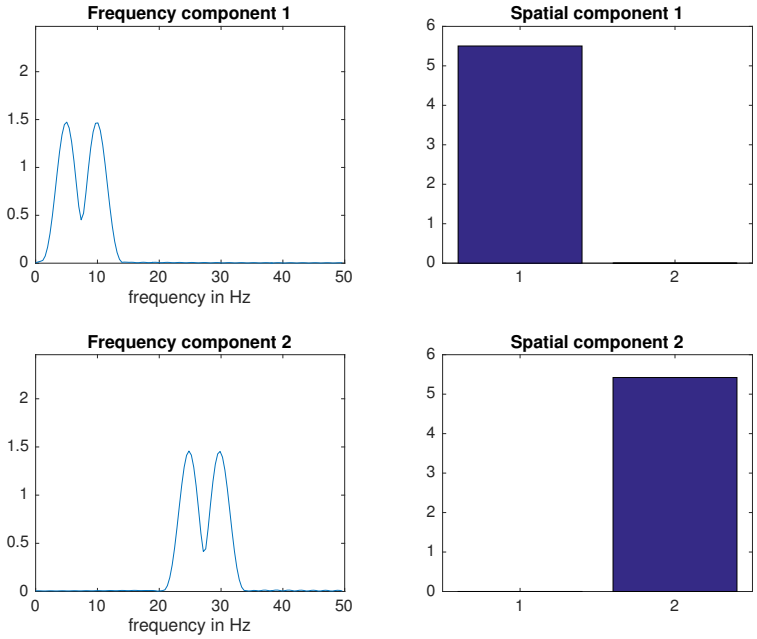
$$\underline{\mathbf{X}} = \sum_{r=1}^{R} \lambda_r \cdot \mathbf{b}_r^{(1)} \circ \mathbf{b}_r^{(2)} \circ \mathbf{b}_r^{(3)} = [\![\underline{\mathbf{D}}; \mathbf{B}^{(1)}, \mathbf{B}^{(2)}, \mathbf{B}^{(3)}]\!] \tag{8}$$

Intuition and physical meaning behind the CPD

$$\begin{aligned} \text{channel}_1 &= 10 \cdot \sin(2\pi t \cdot 20) \\ \text{channel}_2 &= 10 \cdot \sin(2\pi t \cdot 41) \\ \text{channel}_3 &= 10 \cdot \sin(2\pi t \cdot 42) \end{aligned} \tag{9}$$

$$\begin{aligned} \text{channel}_1 &= 10 \cdot \sin(2\pi t \cdot 5) + \\ &\quad 10 \cdot \sin(2\pi t \cdot 10) \\ \text{channel}_2 &= 10 \cdot \sin(2\pi t \cdot 25) + \\ &\quad 10 \cdot \sin(2\pi t \cdot 30) \end{aligned} \tag{10}$$





Intuition and physical meaning behind the CPD

$$
\begin{aligned}
\text{channel}_1 &= 10 \cdot \sin(2\pi t \cdot 5) + 10 \cdot \sin(2\pi t \cdot 12) + 10 \cdot \sin(2\pi t \cdot 15) \\
\text{channel}_2 &= 10 \cdot \sin(2\pi t \cdot 15) + 10 \cdot \sin(2\pi t \cdot 22) + 10 \cdot \sin(2\pi t \cdot 30) \\
\text{channel}_3 &= 10 \cdot \sin(2\pi t \cdot 7) + 10 \cdot \sin(2\pi t \cdot 27) + 10 \cdot \sin(2\pi t \cdot 35) \\
\text{channel}_4 &= 10 \cdot \sin(2\pi t \cdot 6) + 10 \cdot \sin(2\pi t \cdot 13) + 10 \cdot \sin(2\pi t \cdot 40)
\end{aligned}
\tag{11}
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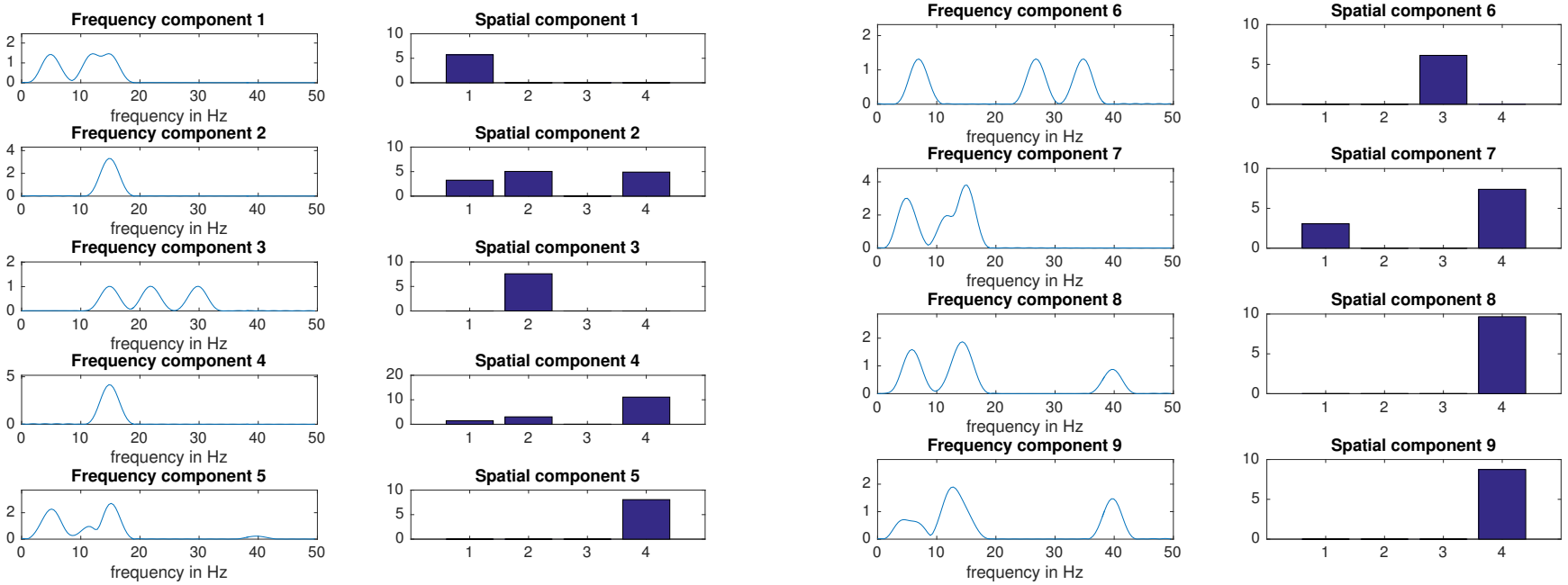

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