Tutorial: Tensor Approximation in Visualization and Computer Graphics

Tensor Decomposition Models

Renato Pajarola, Susanne K. Suter, and Roland Ruiters

University of Zurich UZH

VISUALIZATION AND MULTIMEDIA LAB

universität bonn

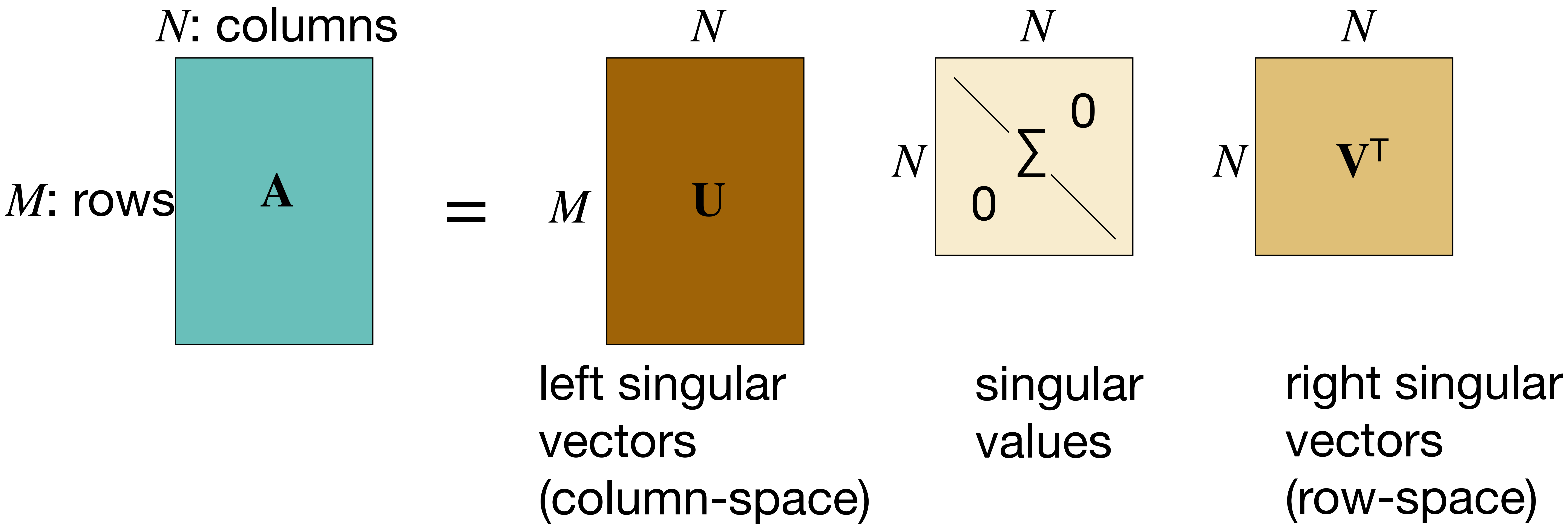
Institute of Computer Science II
Computer Graphics

Data Reduction and Approximation

- A fundamental concept of data reduction is to remove redundant and irrelevant information while preserving the relevant features
  - e.g. through frequency analysis by projection onto pre-defined bases, or extraction of data intrinsic principal components
    - identify spatio-temporal and frequency redundancies
  - maintain strongest and most significant signal components
- Data reduction linked to concepts and techniques of data compression, noise reduction as well as feature extraction and recognition/extraction

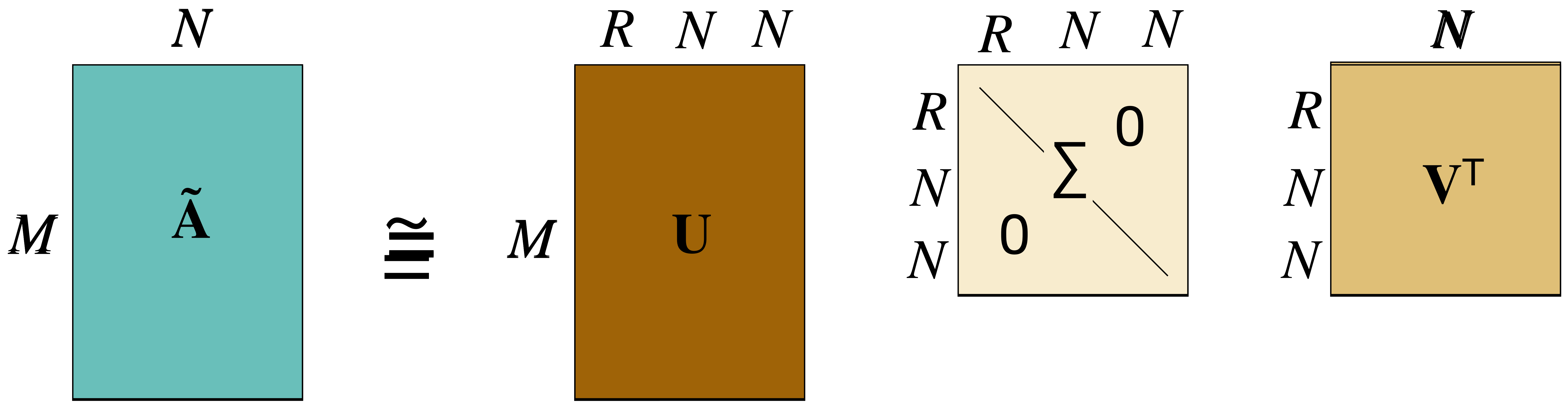
Data Approximation using SVD

- Singular Value Decomposition (SVD) standard tool for matrices, i.e., 2D input datasets
  - see also principal component analysis (PCA)



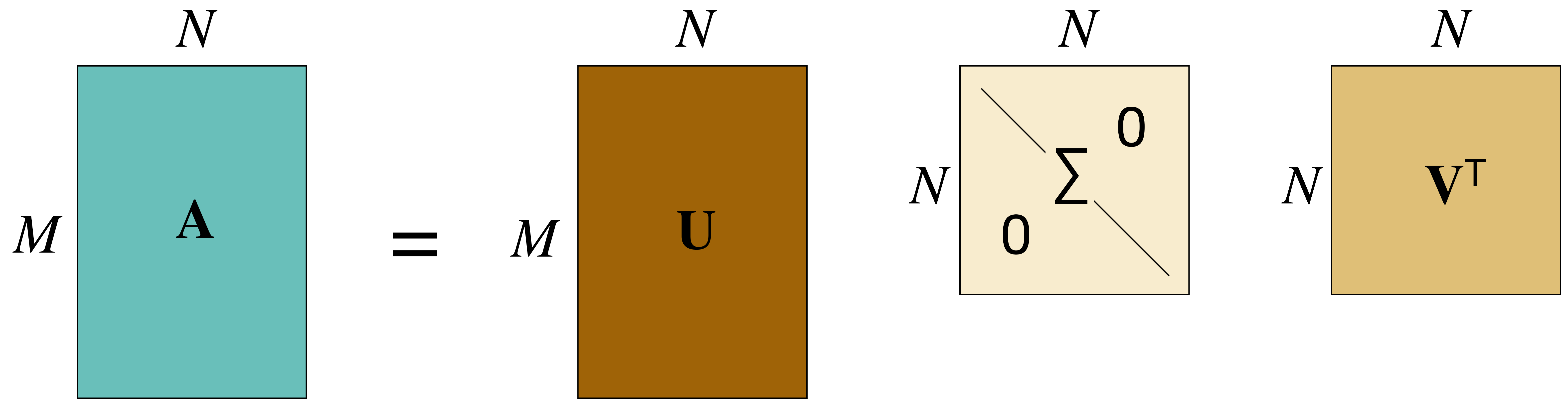
Low-rank Approximation

- Exploit ordered singular values: $s_1 \geq s_2 \geq \ldots \geq s_N$
- Select first r singular values (rank reduction)
  - use only bases (singular vectors) of corresponding subspace

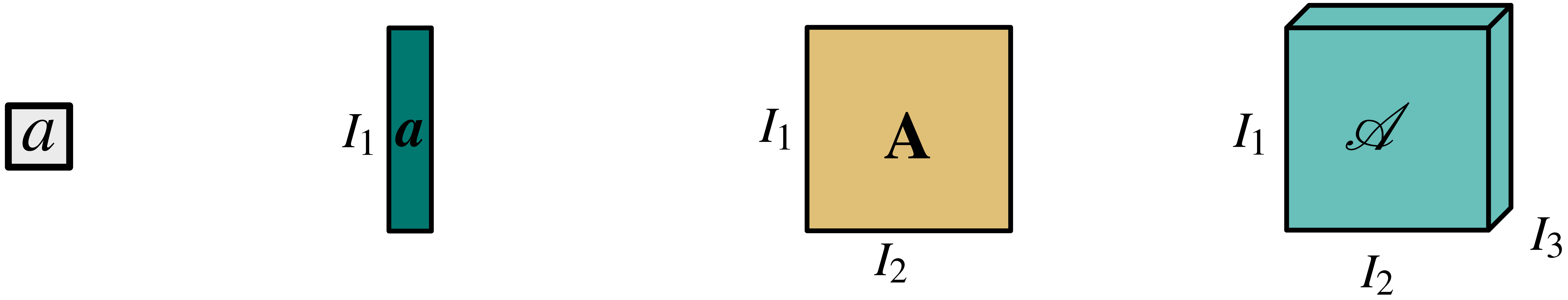


Matrix SVD Properties

- Matrix SVD
  - rank reducibility
  - orthonormal row/column matrices



What is a Tensor?



$\mathscr{A}^{N-\text{th order}} \in \mathbb{R}^{I_1 \times I_2 \cdots \times I_N}$

$i_1 = 1, \ldots, I_1$ $i_2 = 1, \ldots, I_2$ $i_3 = 1, \ldots, I_3$

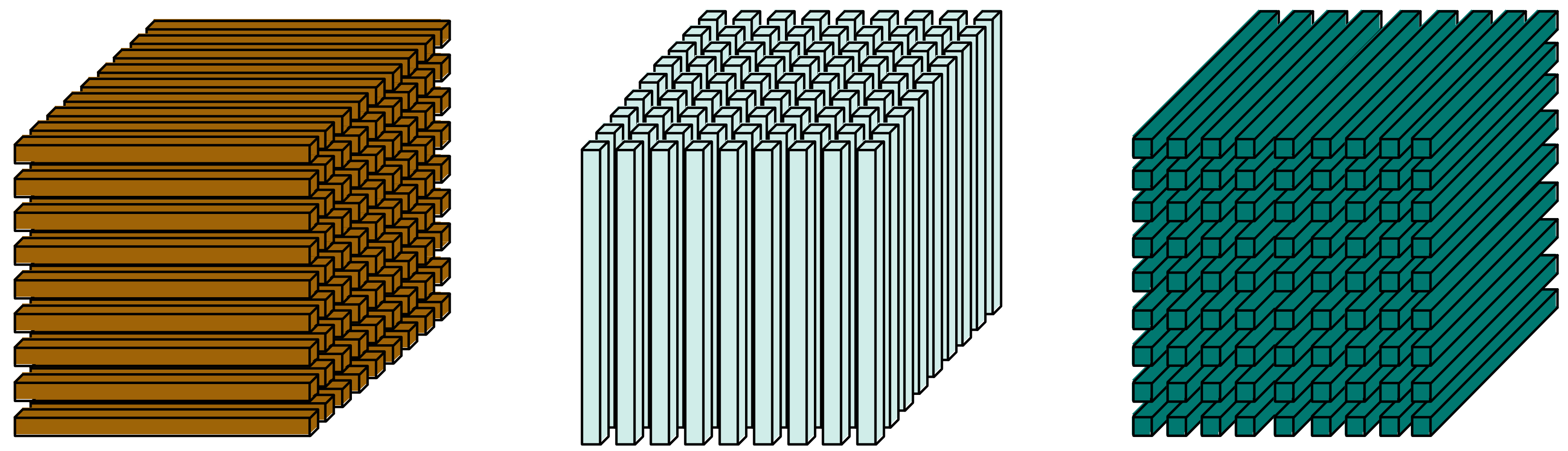
0-order tensor | 1st-order tensor | 2nd-order tensor | 3rd-order tensor | ...

- Data sets are often multidimensional arrays (tensors)
  - images, image collections, video, volume data etc.

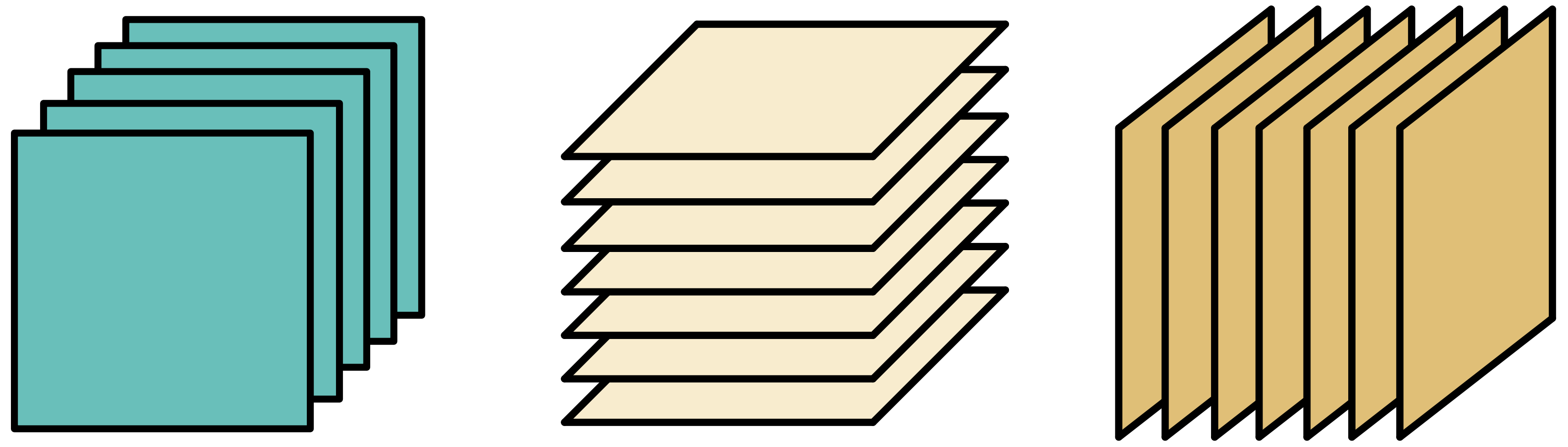
Fibers and Slices

- Individual elements of a vector $\boldsymbol{a}$ are given by a_{i1}, from a matrix $\mathbf{A}$ by $a_{i1,i2}$ and from a tensor $\mathscr{A}$ by $a_{i1,i2,i3}$

- The generalization of rows, columns (and tubes) is a *fiber* in a particular mode

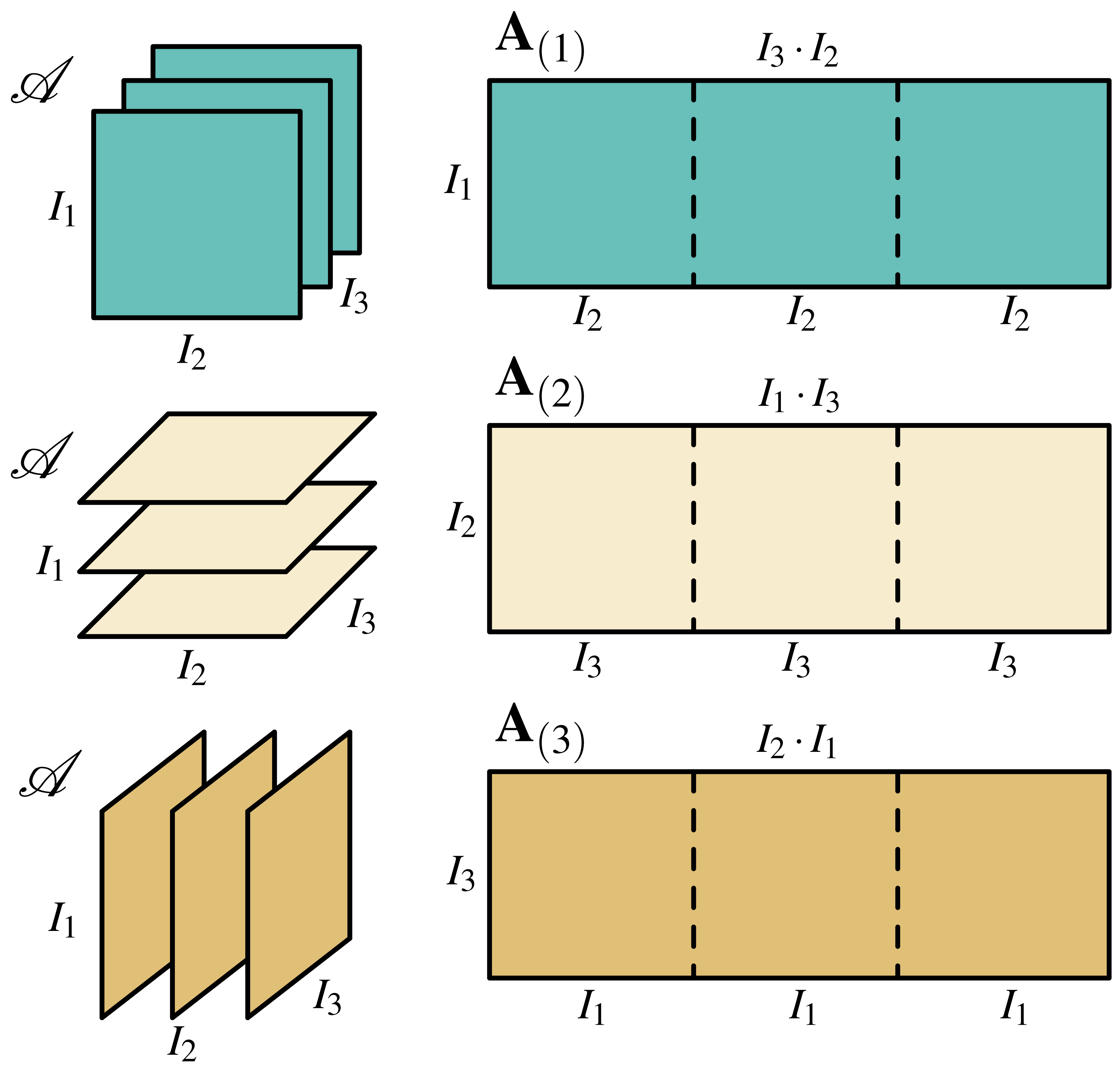


- Two dimensional sections of a tensor are called slices
  - frontal, horizontal and lateral for $\mathscr{A} \in \mathbb{R}^3$



Unfolding and Ranks

- Operations with tensors often performed as matrix operations using unfolded tensor representations
  - different tensor unfolding strategies possible
- Forward cyclic unfolding $\mathbf{A}_{(n)}$ of a 3rd order tensor $\mathscr{A}$ (or 3D volume)
- The n-rank of a tensor is typically defined on an unfolding
  - n-rank $R_n = \text{rank}_n(\mathscr{A}) \;= \text{rank}(\mathbf{A}_{(n)})$
  - multilinear rank-$(R_1, R_2, \ldots, R_N)$ of $\mathscr{A}$

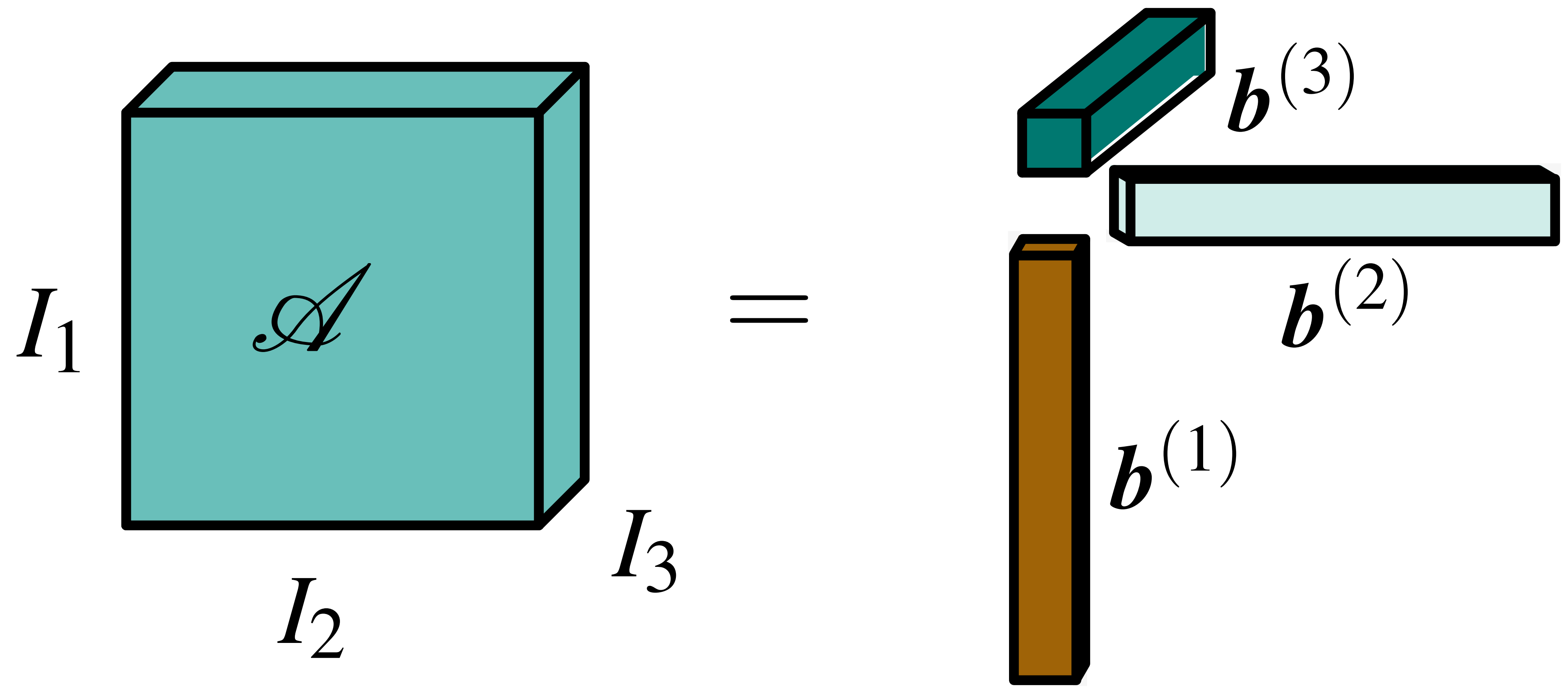


Rank-one Tensor

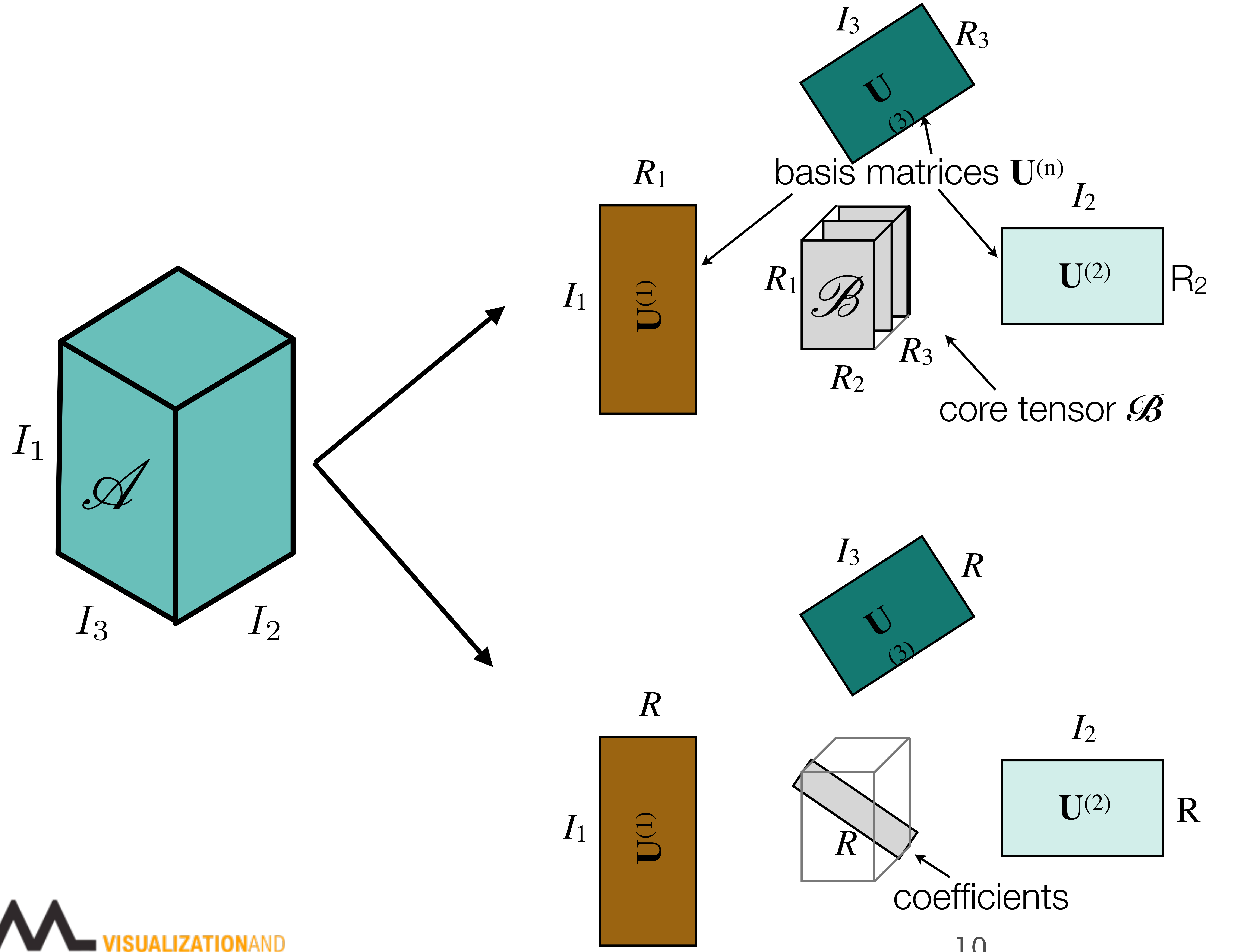
- N-mode tensor $\mathscr{A} \in \mathbb{R}^{I_1 \times \ldots \times I_N}$ that can be expressed as the outer product of N vectors
  - Kruskal tensor

$$\mathscr{A} = \boldsymbol{b}^{(1)} \circ \boldsymbol{b}^{(2)} \circ \cdots \circ \boldsymbol{b}^{(N)}$$

- Useful to understand principles of rank-reduced tensor reconstruction
  - linear combination of rank-one tensors



Tensor Decomposition Models



Tucker

- Three-mode factor analysis (**3MFA/Tucker3**)
  [Tucker, 1964+1966]
- Higher-order SVD (**HOSVD**)
  [De Lathauwer et al., 2000a]

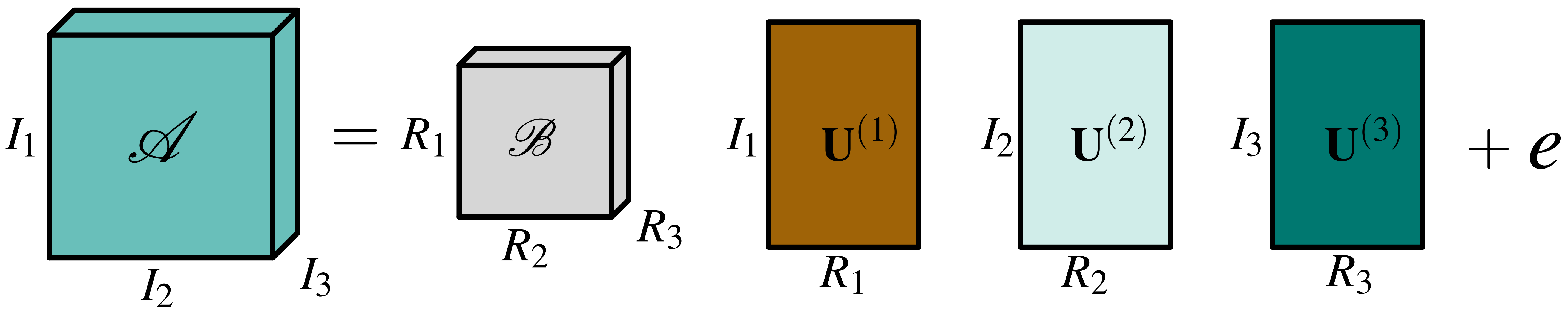
CP

- **PARAFAC** (parallel factors) [Harshman, 1970]
- **CANDECOMP** (CAND) (canonical decomposition)
  [Caroll & Chang, 1970]

Tucker Model

- Higher order tensor $\mathscr{A} \in \mathbb{R}^{I_1 \times \ldots \times I_N}$ represented as a product of a core tensor $\mathscr{B} \in \mathbb{R}^{R_1 \times \ldots \times R_N}$ and N factor matrices $\mathbf{U}^{(n)} \in \mathbb{R}^{I_n \times R_n}$
  - using n-mode products $\times_n$

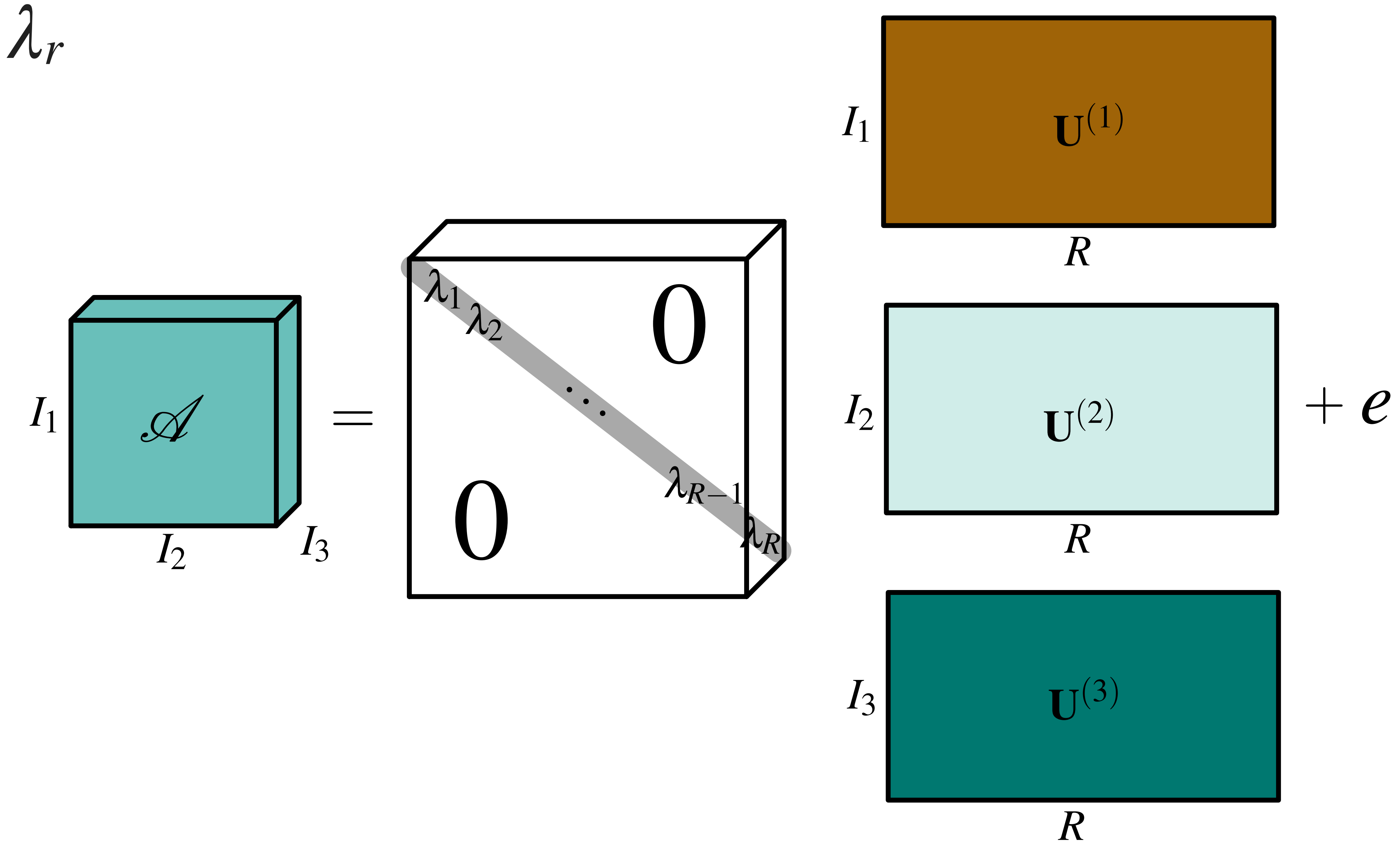
$$\mathscr{A} = \mathscr{B} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \cdots \times_N \mathbf{U}^{(N)} + \varepsilon$$



CANDECOMP-PARAFAC Model

- *Canonical decomposition* or *parallel factor analysis* model (CP)
- Higher order tensor $\mathscr{A}$ factorized into a sum of rank-one tensors
  - normalized column vectors $\boldsymbol{u}_r^{(n)}$ define factor matrices $\mathbf{U}^{(n)} \in \mathbb{R}^{I_n \times R}$ and weighting factors λ_r

$$\mathscr{A} = \sum_{r=1}^{R} \lambda_r \cdot \boldsymbol{u}_r^{(1)} \circ \boldsymbol{u}_r^{(2)} \circ \ldots \boldsymbol{u}_r^{(N)} + \varepsilon$$

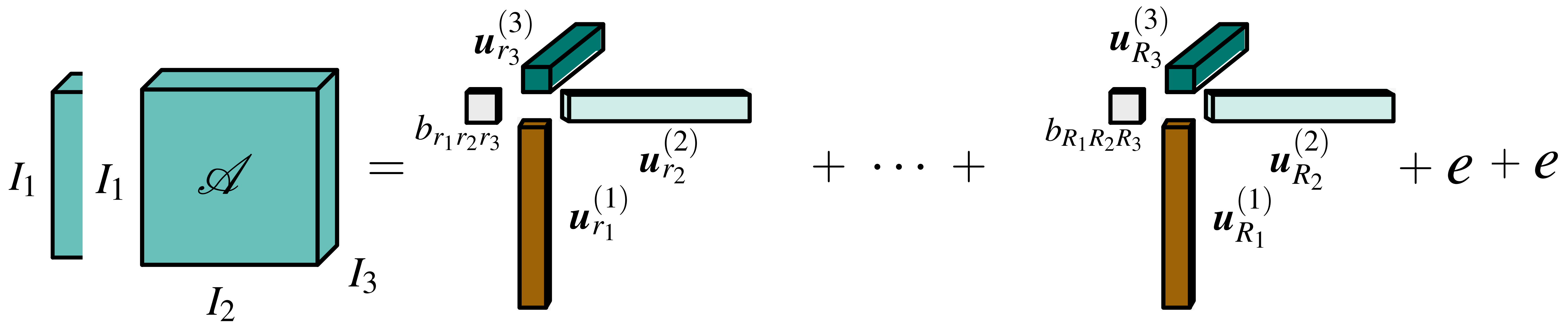


Linear Combination of Rank-one Tensors

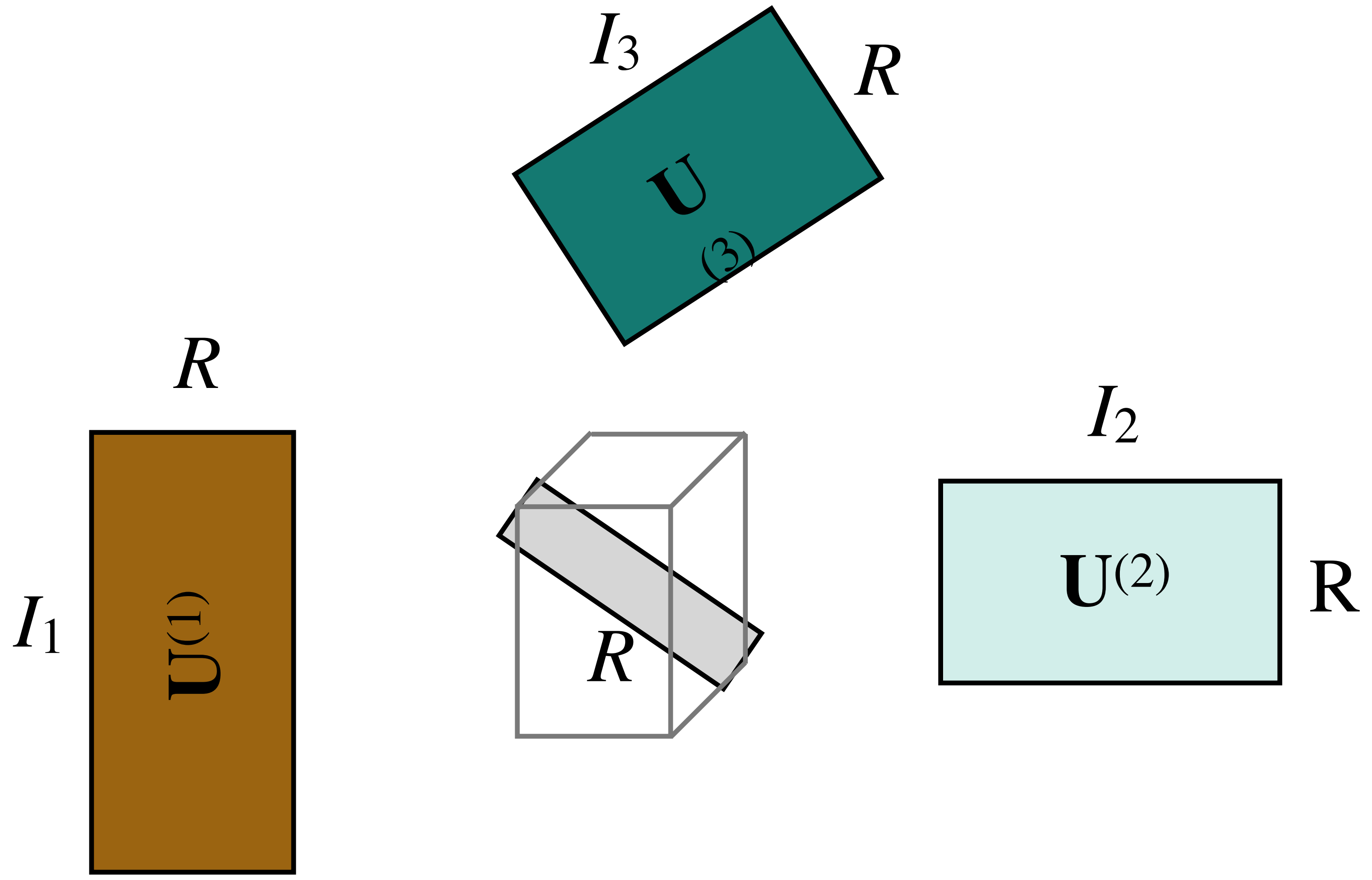
- The CP model is defined as a linear combination of rank-one tensors
- The Tucker model can be interpreted as linear combination of rank-one tensors

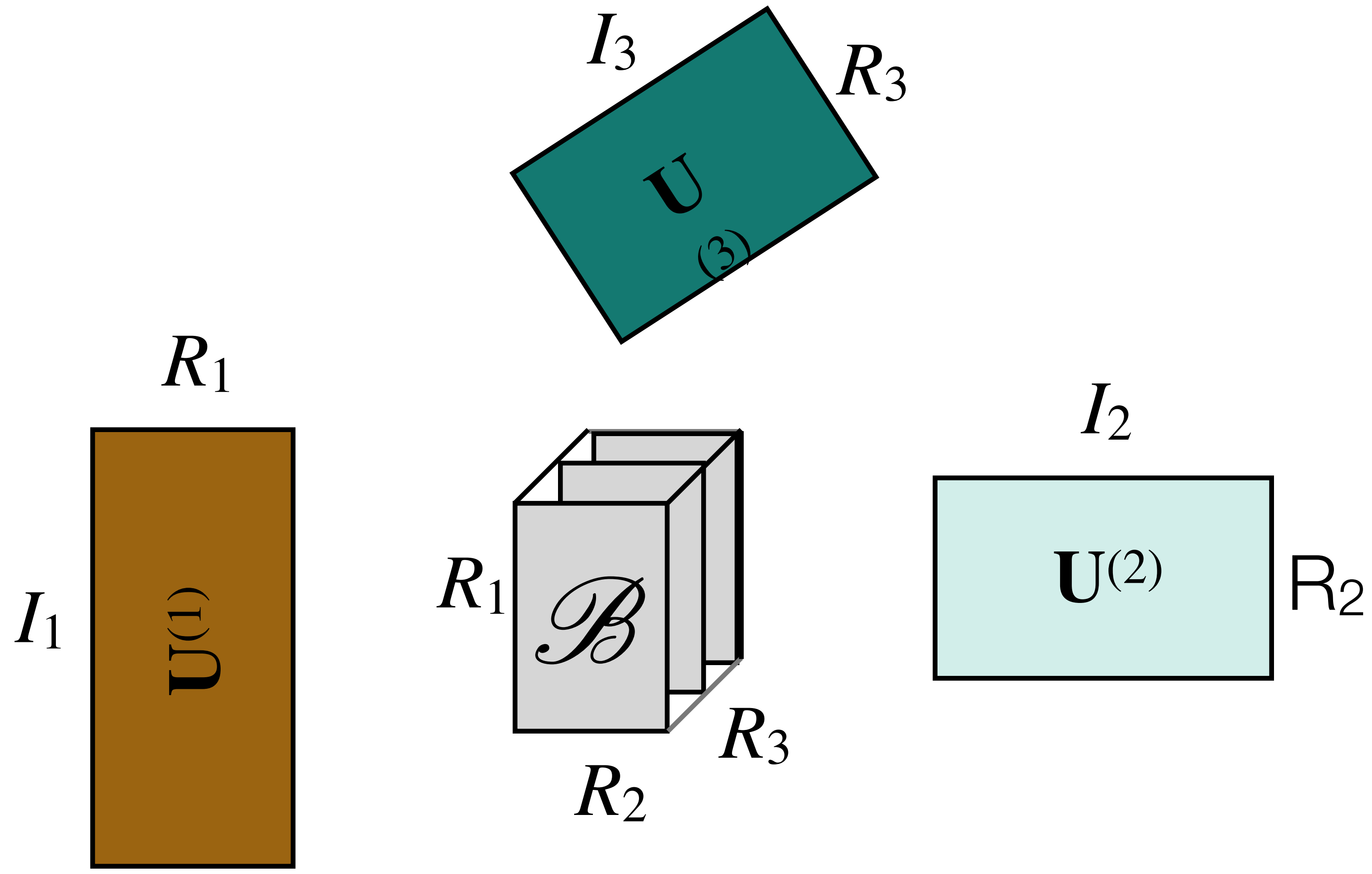
$$\mathscr{A} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_N=1}^{R_N} b_{r_1 r_2 \ldots r_N} \cdot \boldsymbol{u}_{r_1}^{(1)} \circ \boldsymbol{u}_{r_2}^{(2)} \circ \ldots \circ \boldsymbol{u}_{r_N}^{(N)} + \varepsilon$$

$$\mathscr{A} = \sum_{r=1}^{R} \lambda_r \cdot \boldsymbol{u}_r^{(1)} \circ \boldsymbol{u}_r^{(2)} \circ \ldots \circ \boldsymbol{u}_r^{(N)} + \varepsilon$$



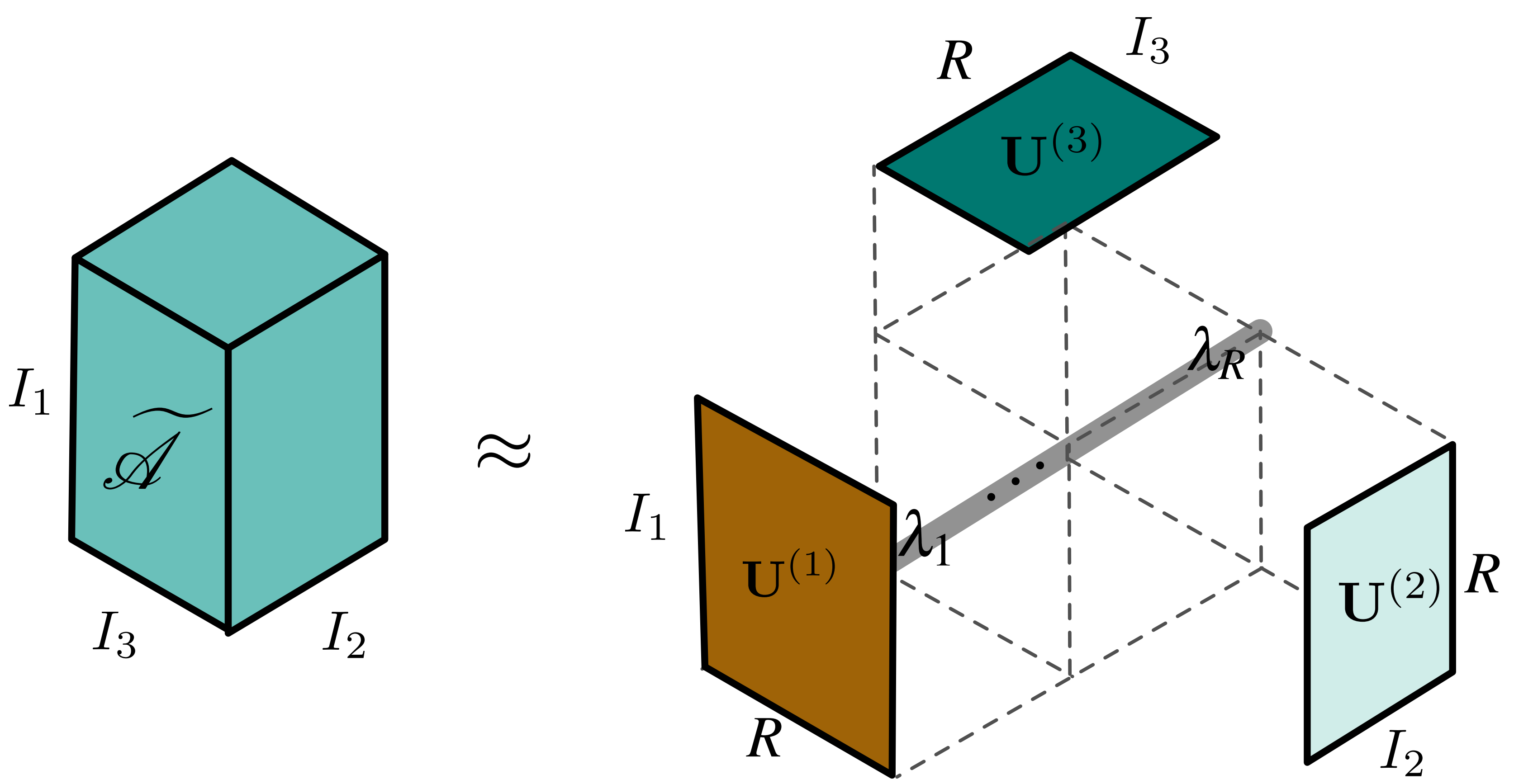
CP a Special Case of Tucker

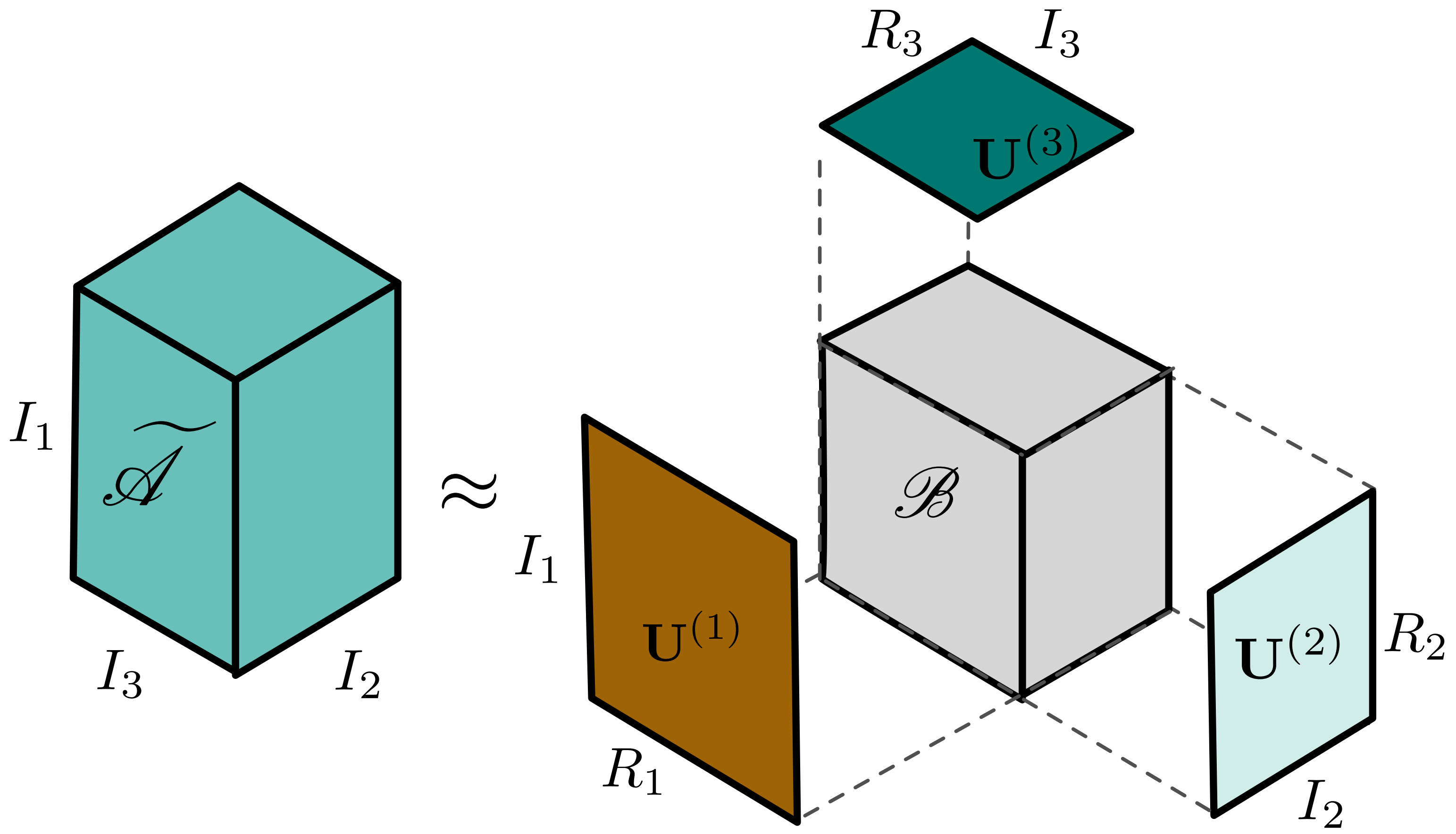




CP

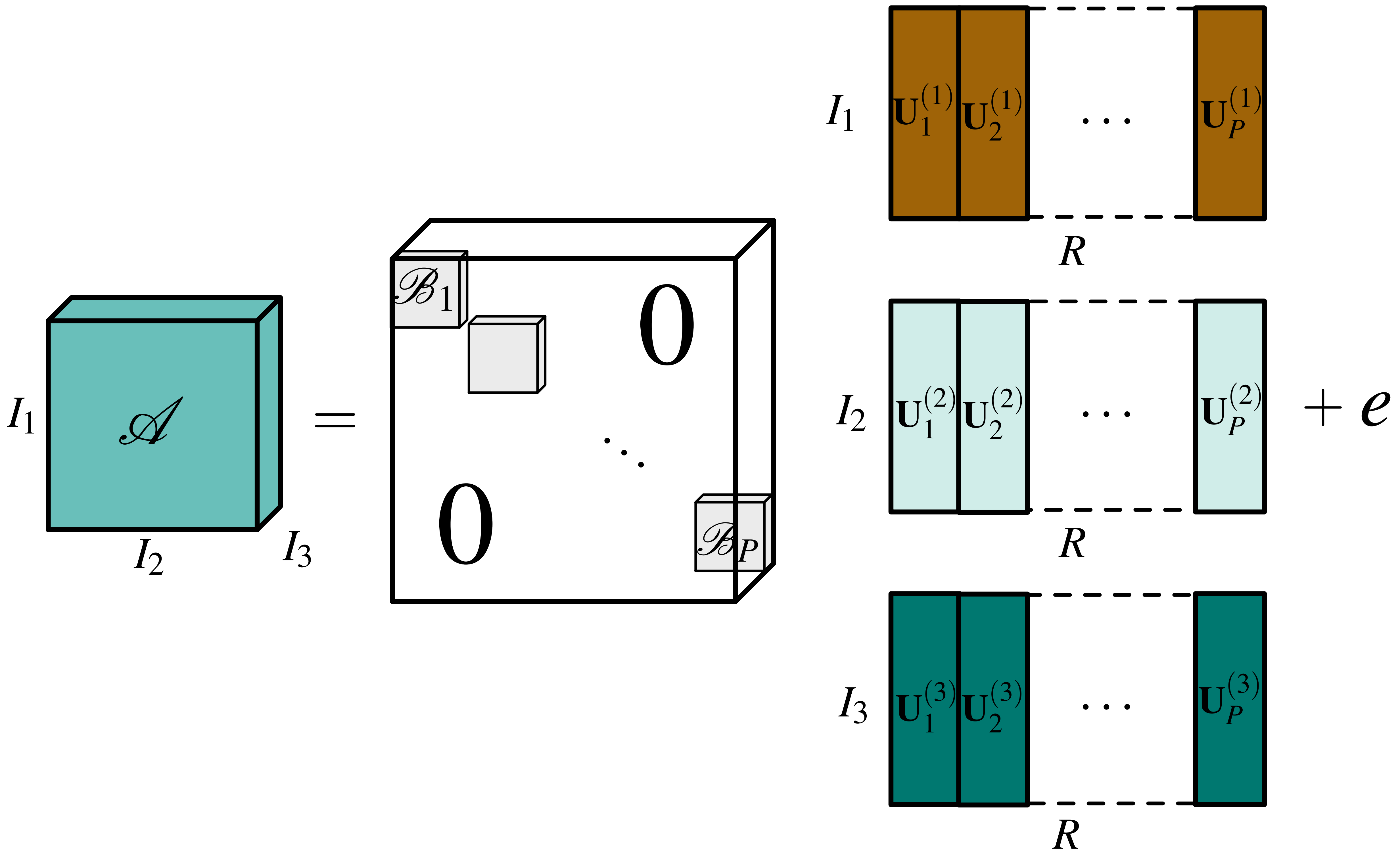
Tucker





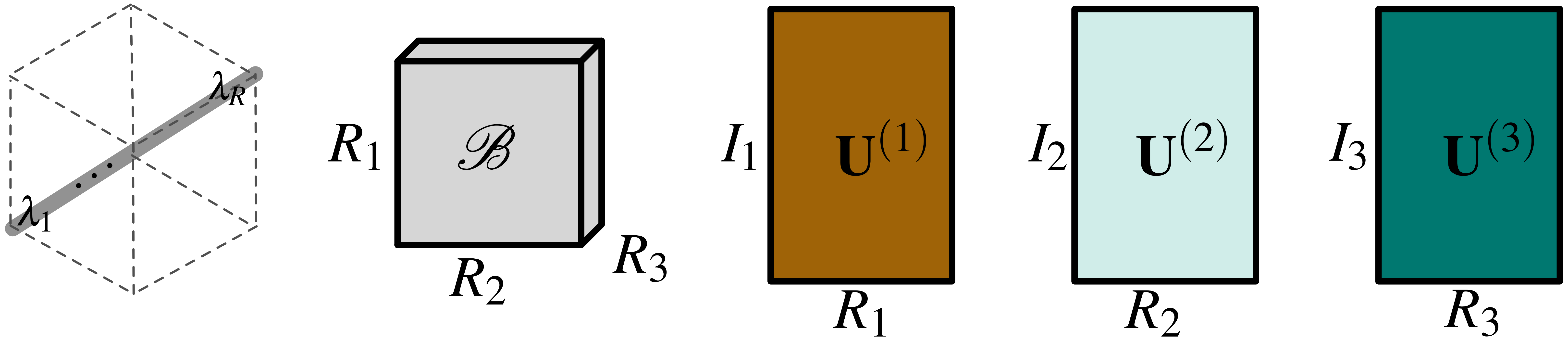
Generalizations

- Any special form of core and corresponding factor matrices
  - e.g. blocks along diagonal



Reduced Rank Approximation

- Full reconstruction using a Tucker or CP model may require excessively many coefficients and wide factor matrices
  - large rank values R (CP), or $R_1, R_2 \dots R_N$ (Tucker)
- Quality of approximation increases with the rank, and number of column vectors of the factor matrices
  - best possible fit of these bases matrices discussed later

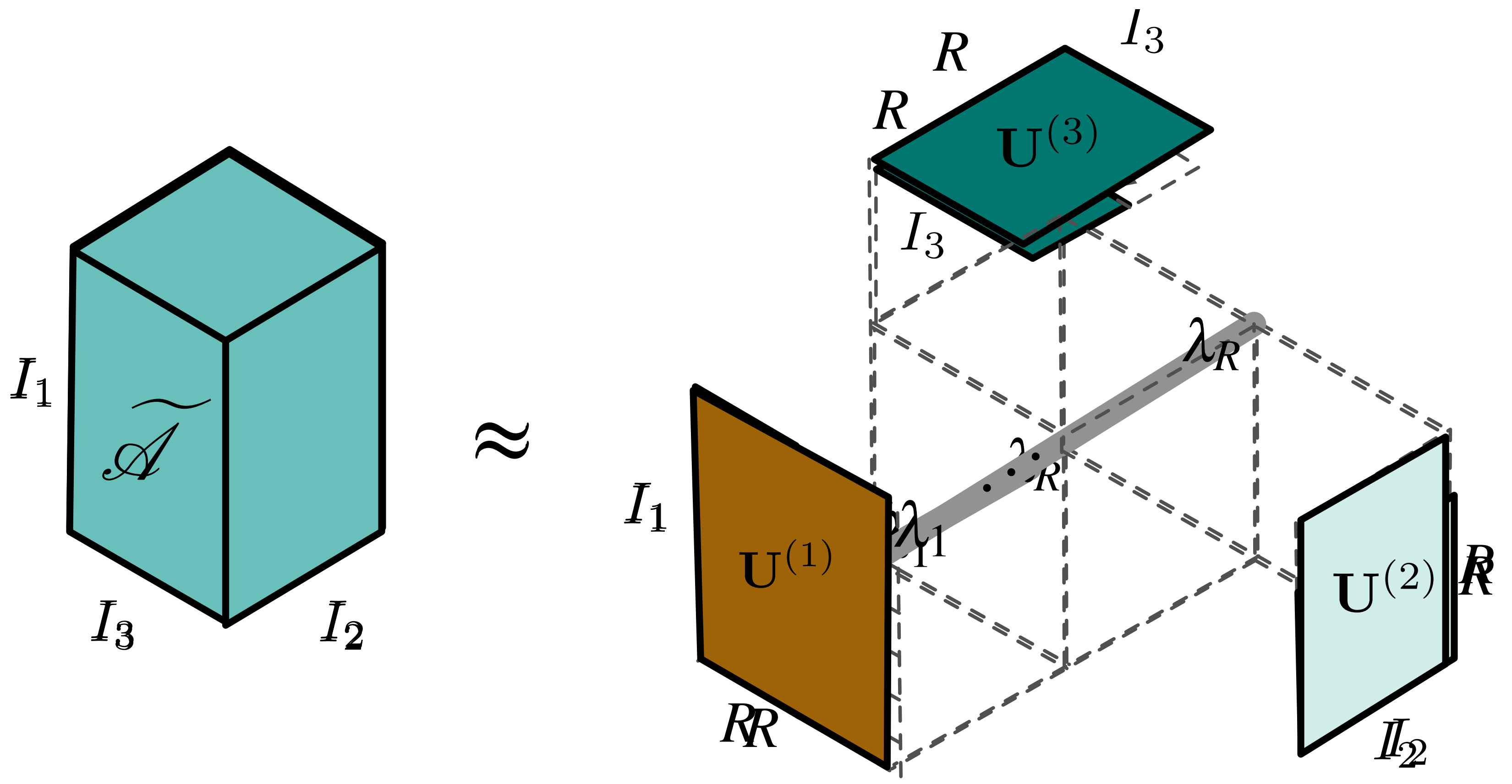


VISUALIZATIONANDMULTIMEDIALAB

universitätbonn

Rank-R Approximation

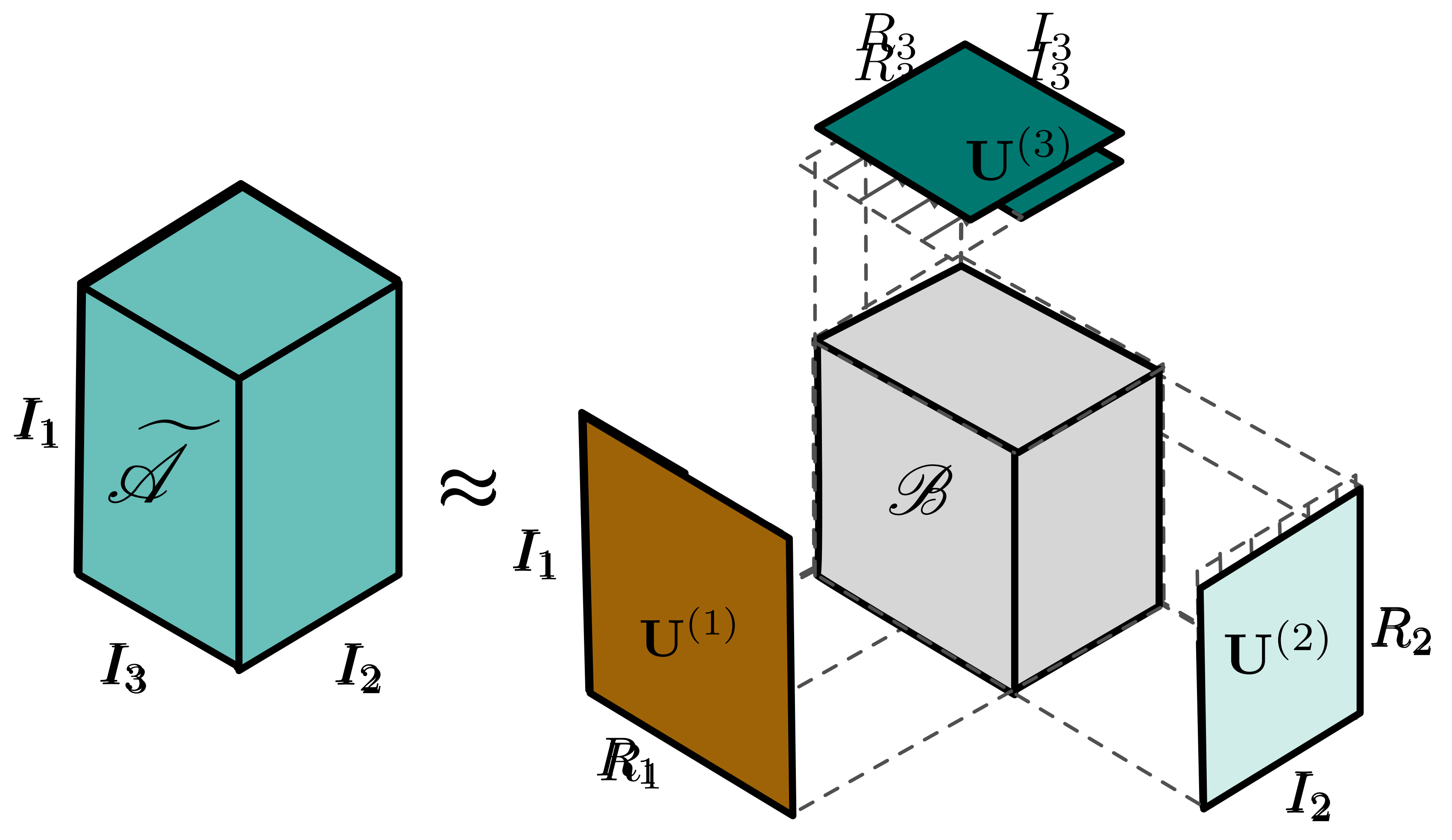
- Approximation of a tensor as a linear combination of ranke-one tensors using a limited number R of terms
  - CP model of limited rank R



$$\widetilde{\mathscr{A}} = \sum_{r=1}^{R} \lambda_r \cdot \boldsymbol{u}_r^{(1)} \circ \boldsymbol{u}_r^{(2)} \circ \ldots \boldsymbol{u}_r^{(N)}$$

Rank-$(R_1, R_2, \ldots, R_N)$ Approximation

- Decomposition into a tensor with reduced, lower multilinear $\text{rank}(R_1, R_2, \ldots, R_N)$
  - $\text{rank}_n(\widetilde{\mathscr{A}}) = R_n \leq \text{rank}_n(\mathscr{A}) = \text{rank}(\mathbf{A}_{(n)})$
- $\boldsymbol{n}$-mode products of factor matrices and core tensor in a given reduced rank space
  - Tucker model with limited ranks R_i



$$\widetilde{\mathscr{A}} = \mathscr{B} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \cdots \times_N \mathbf{U}^{(N)}$$

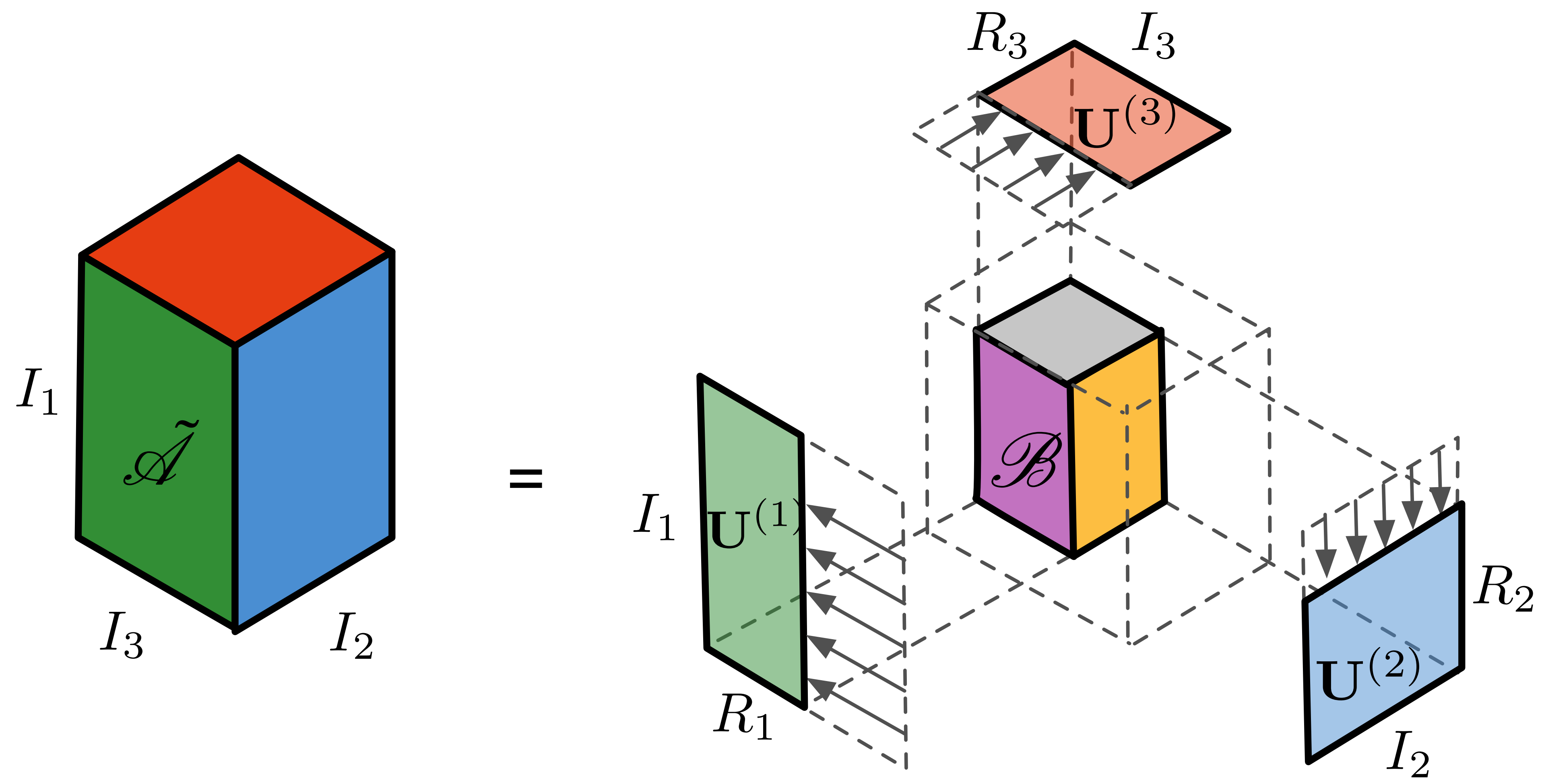
VISUALIZATION AND MULTIMEDIA LAB

universität bonn

Best Rank Approximation

- Rank reduced approximation that minimizes least-squares cost
  - $$\widetilde{\mathscr{A}} = \arg\min(\widetilde{\mathscr{A}}) \left\| \mathscr{A} - \widetilde{\mathscr{A}} \right\|^2$$

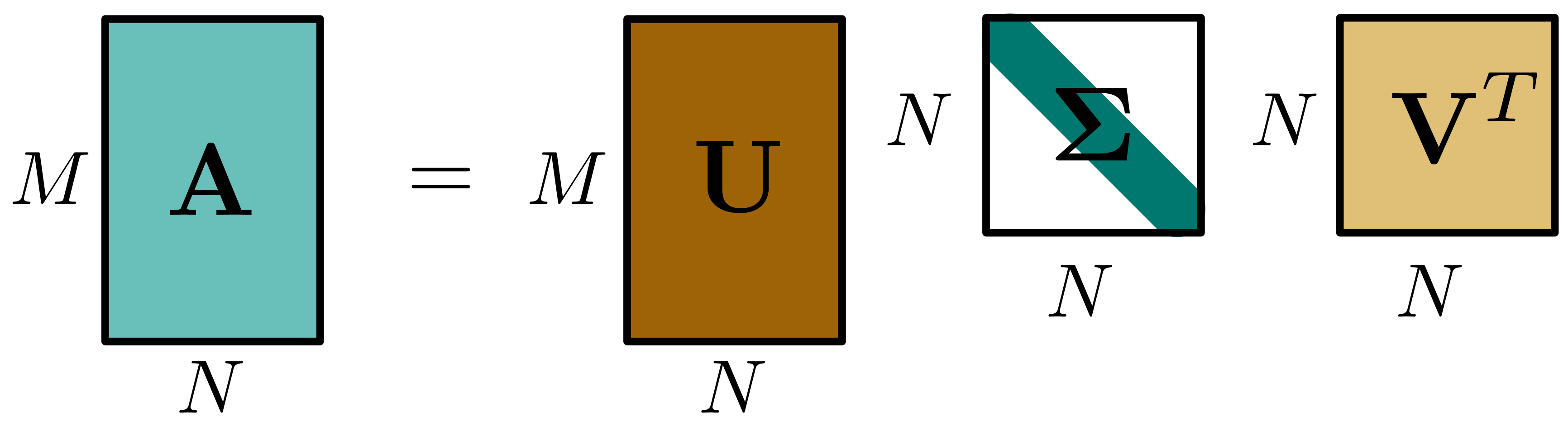
- Alternating least squares (ALS) iterative algorithm that converges to a minimum approximation error based on the Frobenius norm $\|\ldots\|_F$
  - rotation of components in basis matrices



$$\widetilde{\mathscr{A}} = \mathscr{B} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)}$$

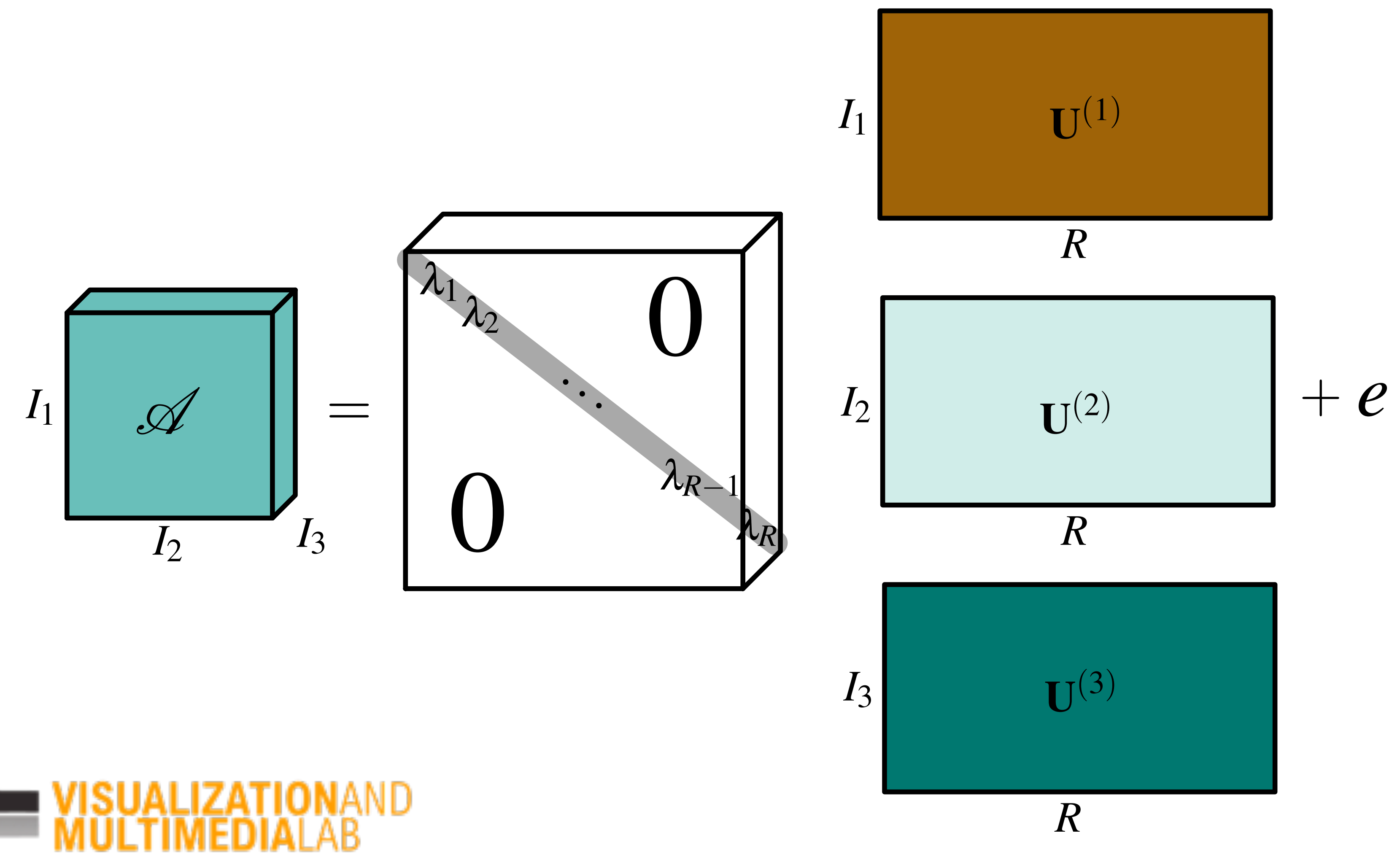
typical high-quality data reduction:
$R_k \leq I_k / 2$

Generalization of the Matrix SVD

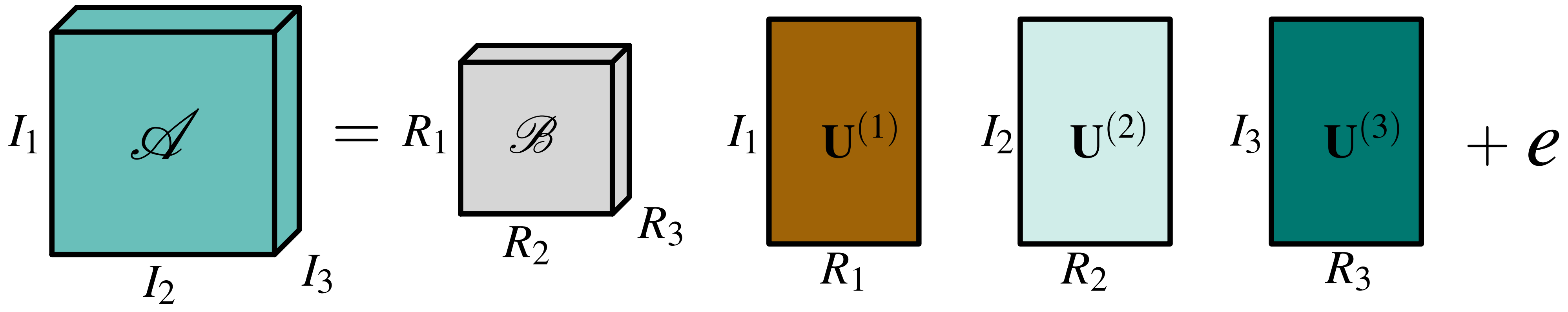


higher orders

CP model



Tucker model



Tutorial: Tensor Approximation in Visualization and Computer Graphics

TA Properties and Features

Renato Pajarola, Susanne K. Suter, and Roland Ruiters

University of Zurich[UZH]

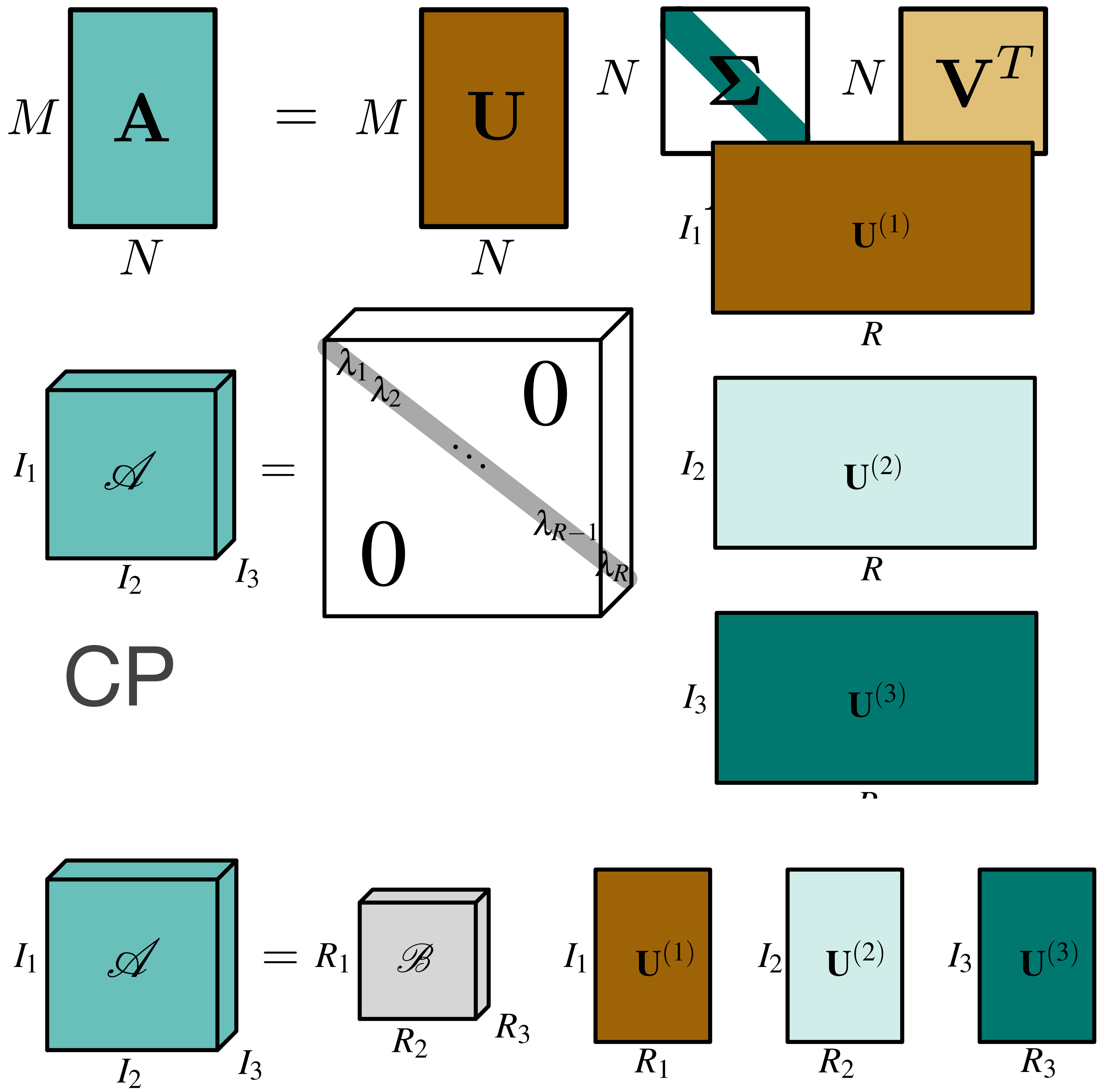
VISUALIZATION AND MULTIMEDIA LAB

universität bonn

Institute of Computer Science II
Computer Graphics

Properties of Higher Order TA

- Matrix SVD (~PCA)
  - unique
  - rank-R decomposition
  - orthonormal row-space and column-space vectors
- Higher-order tensor decomposition
  - CP model preserves rank-R decomposition
  - all-orthogonal Tucker model preserves orthonormal row-space and column-space vectors



Tucker

VISUALIZATIONANDMULTIMEDIALAB

universitätbonn

Matrix and Tensor Rank Definitions

- Matrix has unique equal column and row ranks
  - result of SVD
- The n-ranks $R_n = \mathrm{rank}_n(\mathscr{A})$ of a tensor $\mathscr{A}$ may all be different
  - different unfoldings $\mathbf{A}_{(n)}$ give rise to different n-ranks $\mathrm{rank}(\mathbf{A}_{(n)})$
- Matrix rank concept is not uniquely defined for higher order tensors
  - n-rank R_n
  - multilinear rank-$(R_1, R_2, \ldots, R_n)$
  - tensor rank $R = \mathrm{rank}(\mathscr{A})$

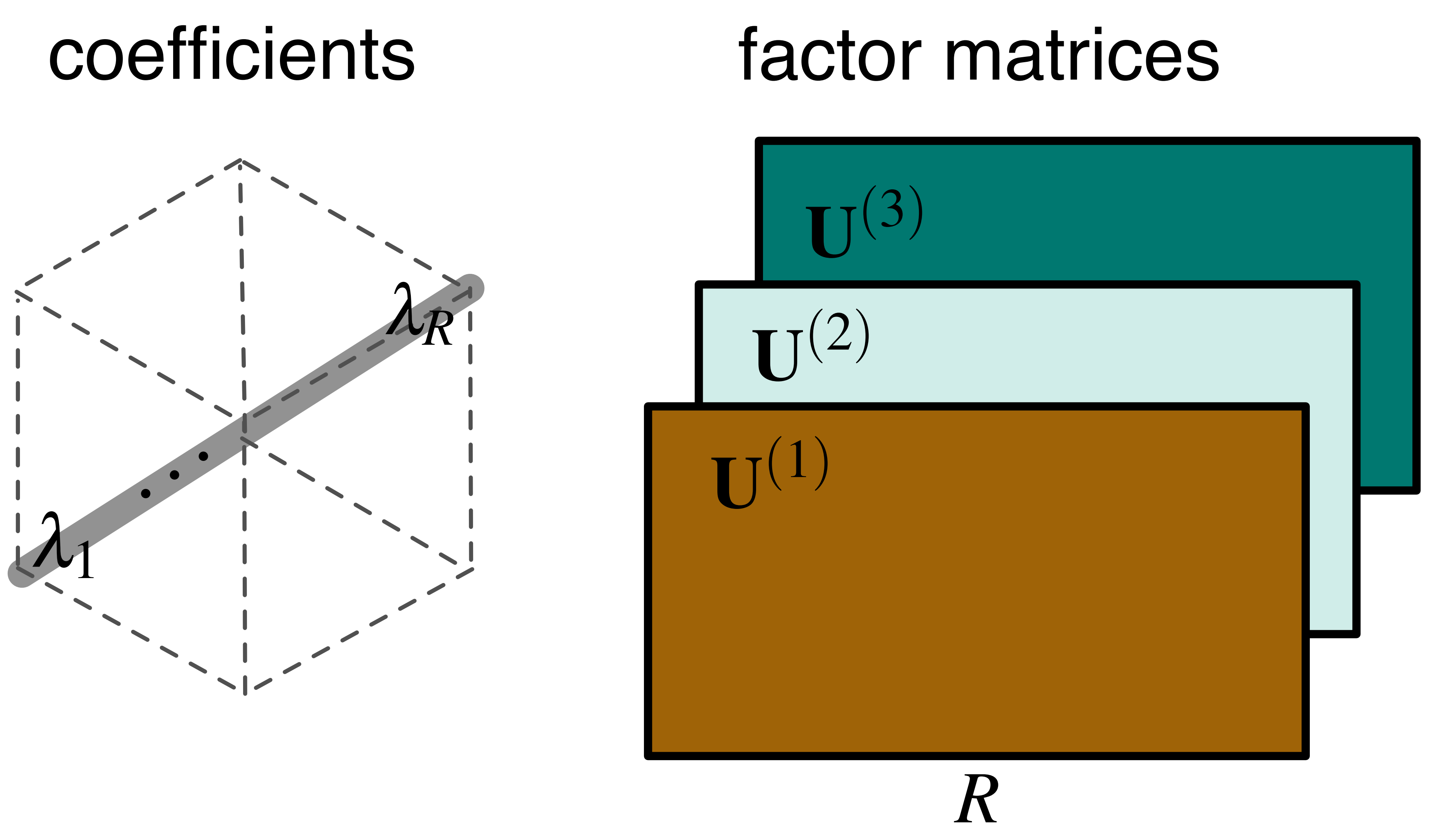
Tensor Rank R

- The ***tensor rank*** $R = \mathrm{rank}(\mathscr{A})$ is the minimal number of rank-one tensors $\mathscr{A}_i$ that yield $\mathscr{A}$ in a linear combination
  - $\mathscr{A}_i$ are rank-one tensors, defined by outer product of N vectors
- Equal to the column and row rank for matrices
- Not necessarily equal to any n-rank R_n of a tensor
  - and it holds that $R \geq R_n$

Rank-R Decomposition

- Minimal number R of rank-one tensors $\mathscr{A}_i$ that yield $\mathscr{A}$ in a linear combination, $\mathscr{A} = \lambda_1 \mathscr{A}_1 + \lambda_2 \mathscr{A}_2 + \ldots + \lambda_R \mathscr{A}_R$
- CP model allows a direkt rank-R decomposition with respect to the *tensor rank* R

$$\mathscr{A} = \sum_{r=1}^{R} \lambda_r \cdot \boldsymbol{u}_r^{(1)} \circ \boldsymbol{u}_r^{(2)} \circ \cdots \circ \boldsymbol{u}_r^{(N)}$$



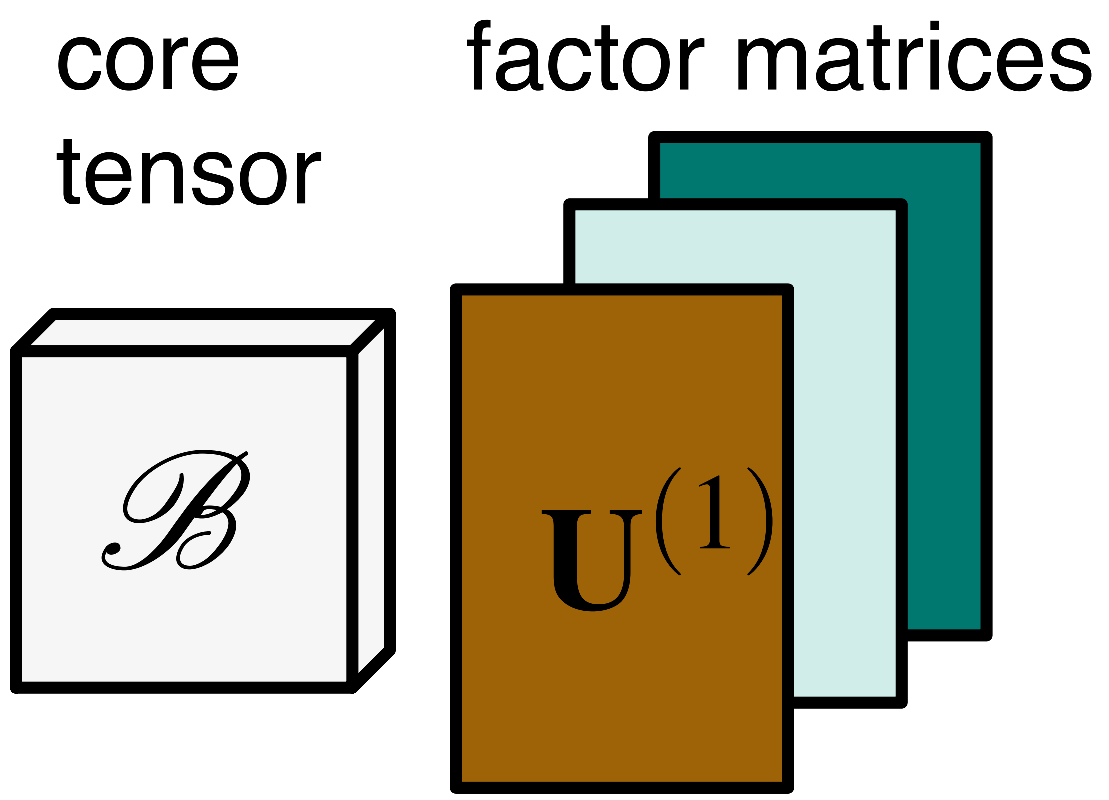
Uniqueness

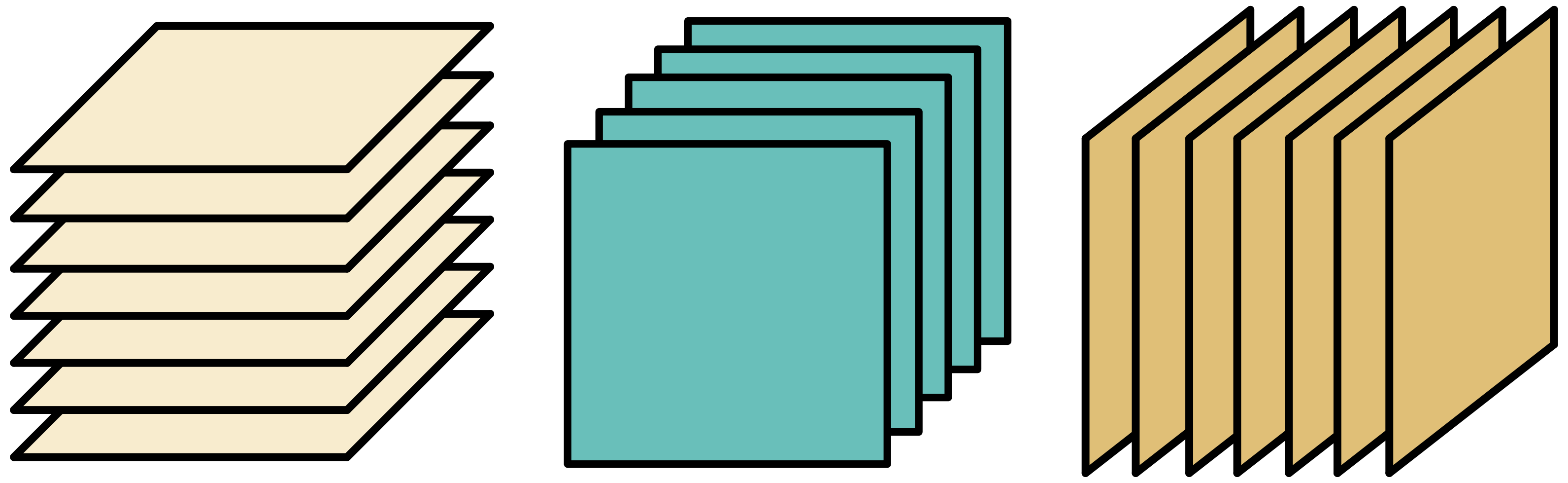
- Unique if it is the only possible decomposition
  - except for indeterminacies of scaling and permutations
- Rank-R decompositions of higher-order tensors are often unique
- Matrix rank decompositions are not generally unique,
  except e.g. for the SVD
  - due to the orthogonality constraints, and
  - the diagonal matrix of ordered singular values
- The CP decomposition is unique under weaker conditions (than the SVD)
  - non-orthogonal factor matrices
- The Tucker decomposition is not unique

[Kolda and Bader, 2009]

Orthonormality

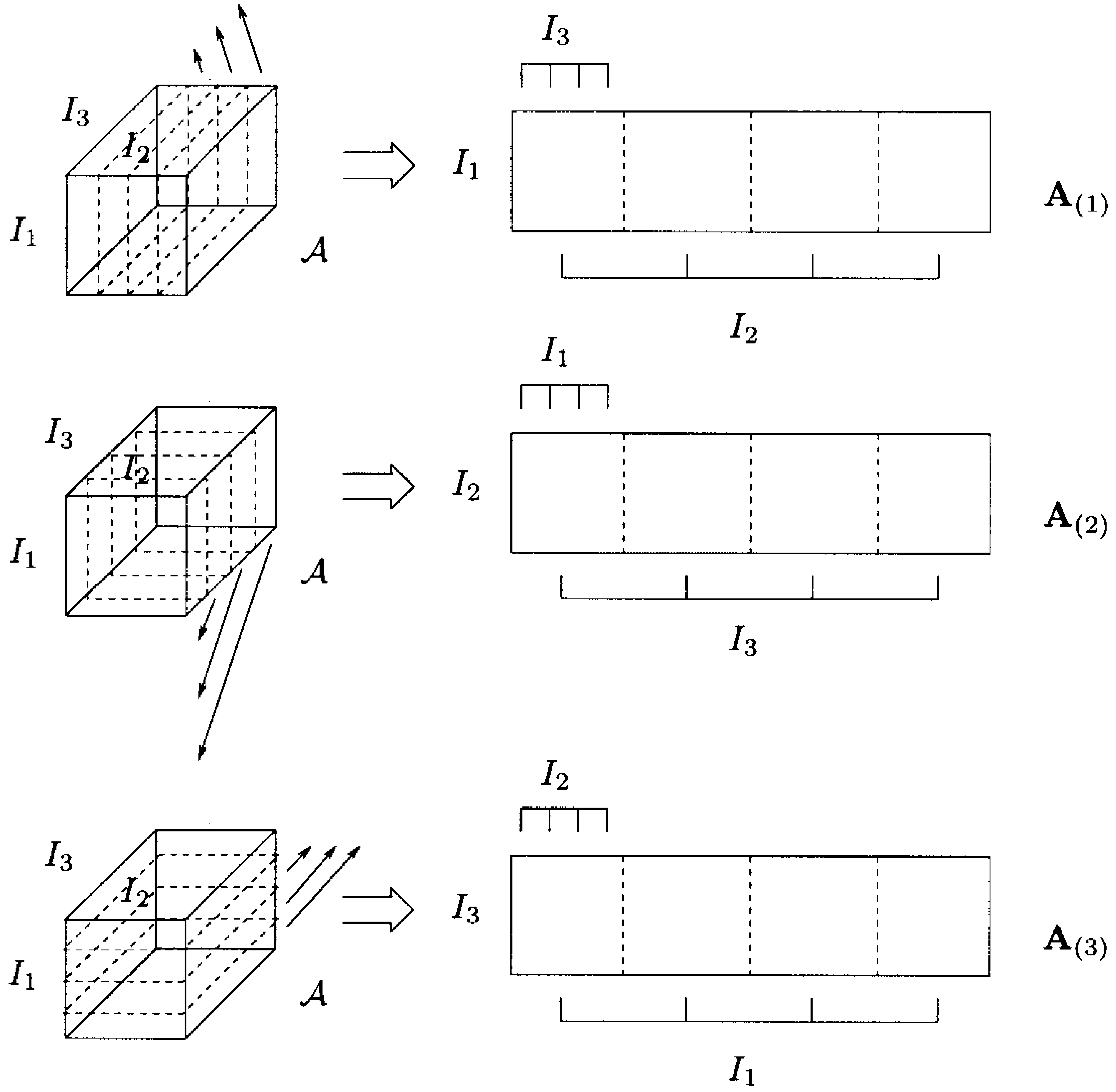
- Matrix SVD generates orthonormal bases $\mathbf{U}$ and $\mathbf{V}$
- A Tucker model can be formed with orthonormal factor matrices
  - all-orthogonal Tucker core tensor $\mathscr{B}$
- All-orthogonality example for third-order tensor:
  - horizontal matrices are mutually orthogonal with respect to the scalar product of matrices
    - the sum of the products of the corresponding entries vanishes
  - the same holds for all frontal slices and lateral slices
    - see De Lathauwer et al., 2000a





Higher-Order SVD (HOSVD)

Tensor unfolding



HOSVD algorithm

- SVD on every mode's tensor unfolding $\mathbf{A}_{(n)}$
  - set basis factor matrices $\mathbf{U}^{(n)}$ as R leading left singular vectors of $\mathbf{A}_{(n)}$
- Derive core $\mathcal{B}$ from original data and inverse factor matrices
  - defines a Tucker model with $\mathcal{B}$, $\mathbf{U}^{(n)}$

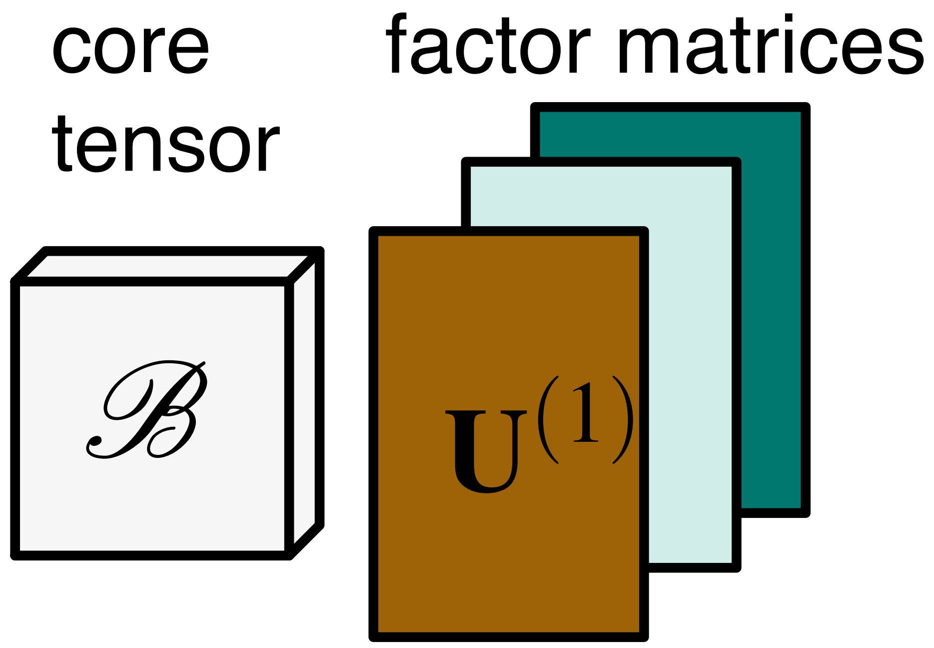
$$\mathcal{B} = \mathcal{A} \times_1 \mathbf{U}^{(1)^{-1}} \times_2 \mathbf{U}^{(2)^{-1}} \times_3 \mathbf{U}^{(3)^{-1}}$$

HOSVD: Lathauwer et al., 2000a

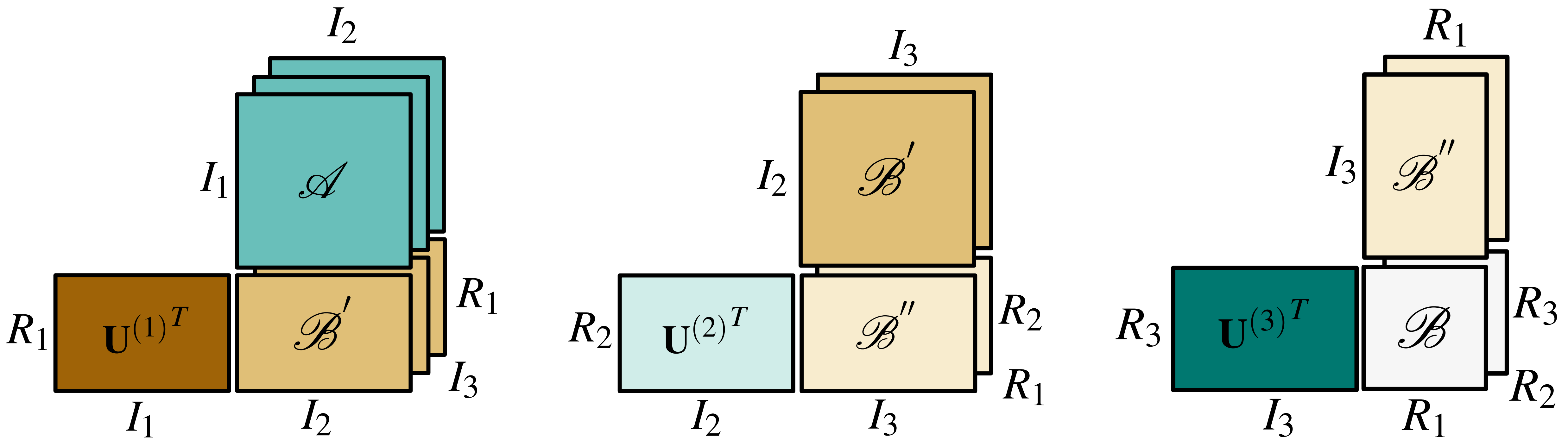
Tucker Core

- Tucker column vectors of factor matrices $\mathbf{U}^{(n)}$ are often defined to be orthonormal
- Core tensor $\mathscr{B}$ represents projection of data $\mathscr{A}$ onto its factor matrices $\mathbf{U}^{(n)}$, thus is a representation in new bases
  - computed using transposes for orthogonal factor matrices

$$\mathscr{B} = \mathscr{A} \times_1 \mathbf{U}^{(1)^{\mathrm{T}}} \times_2 \mathbf{U}^{(2)^{\mathrm{T}}} \times_3 \mathbf{U}^{(3)^{\mathrm{T}}}$$



- Optimized order of computation

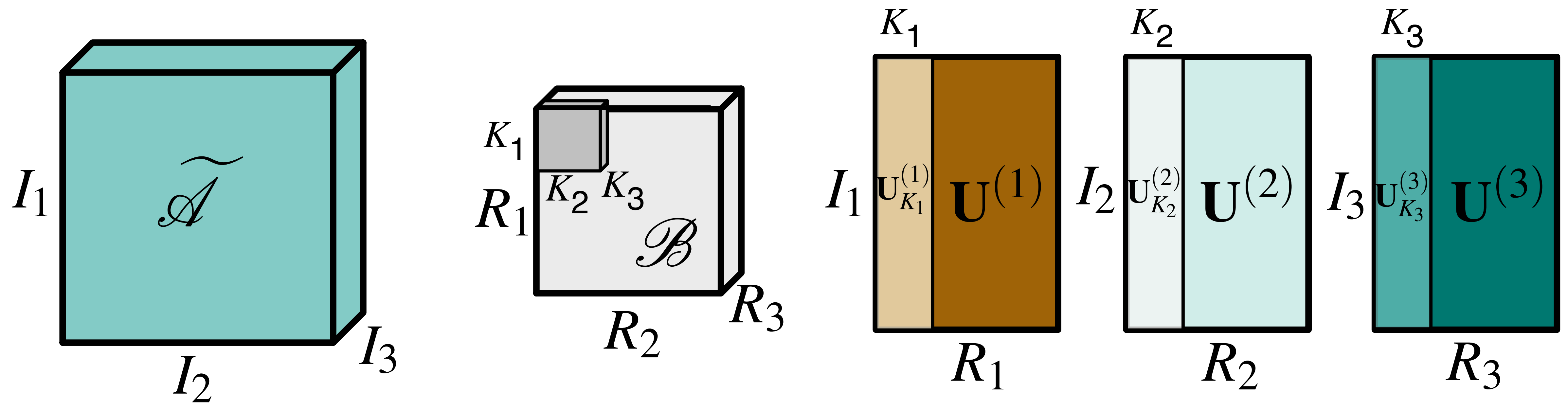


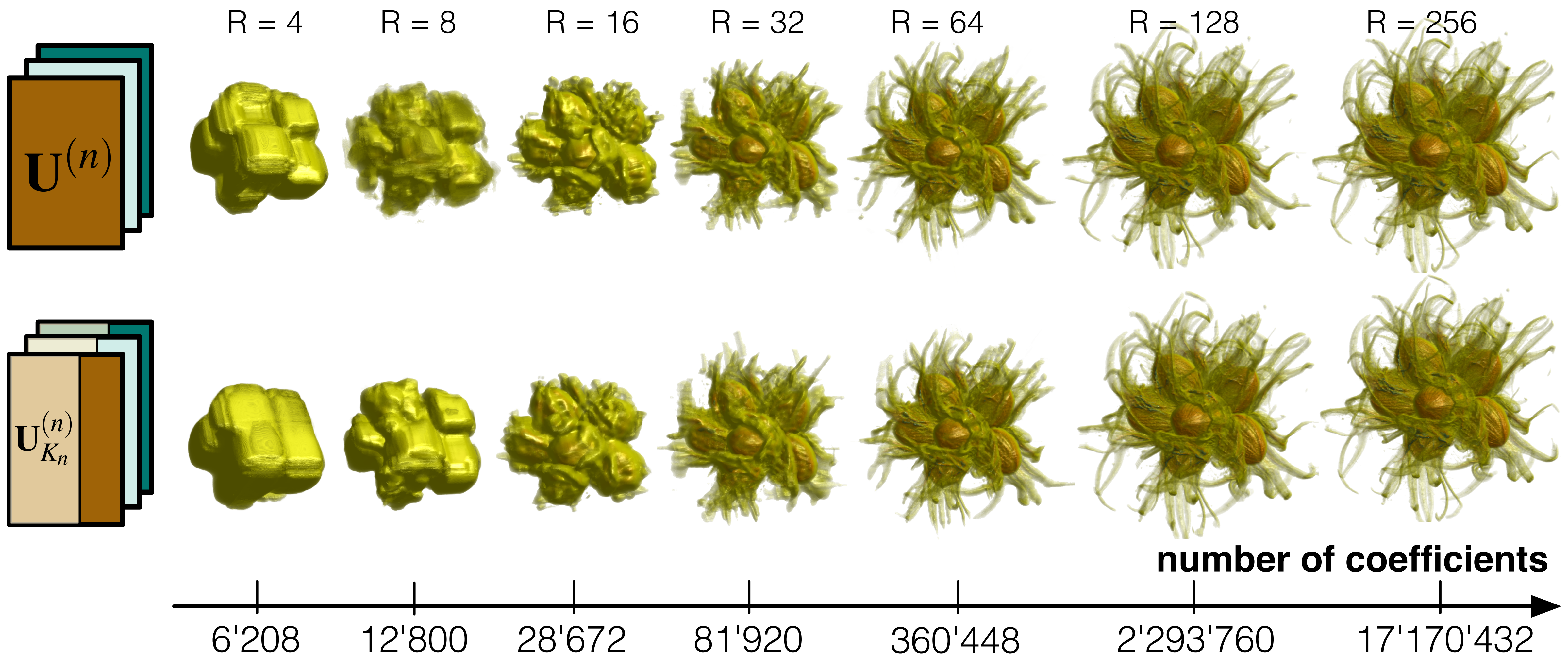
VISUALIZATION AND MULTIMEDIA LAB

universität bonn

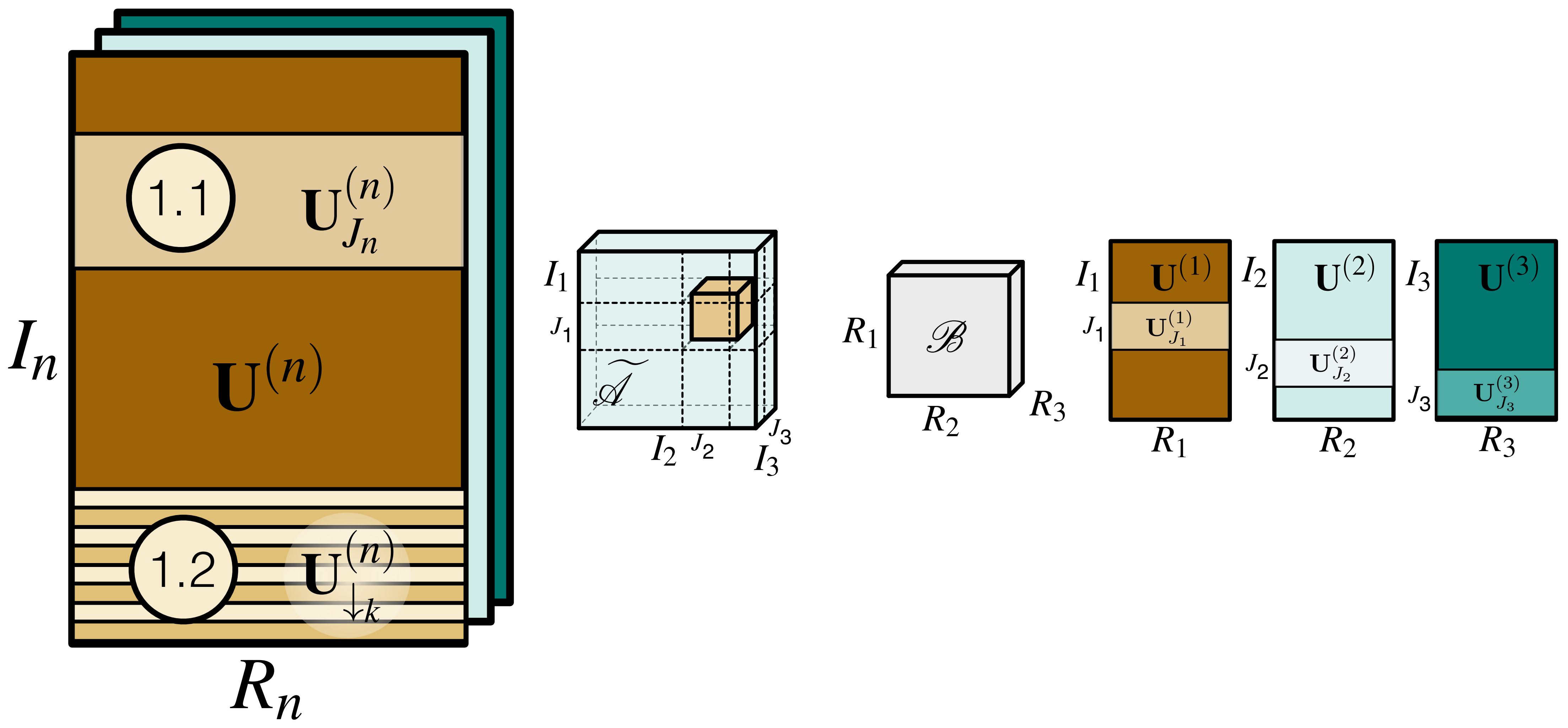
Rank Truncation

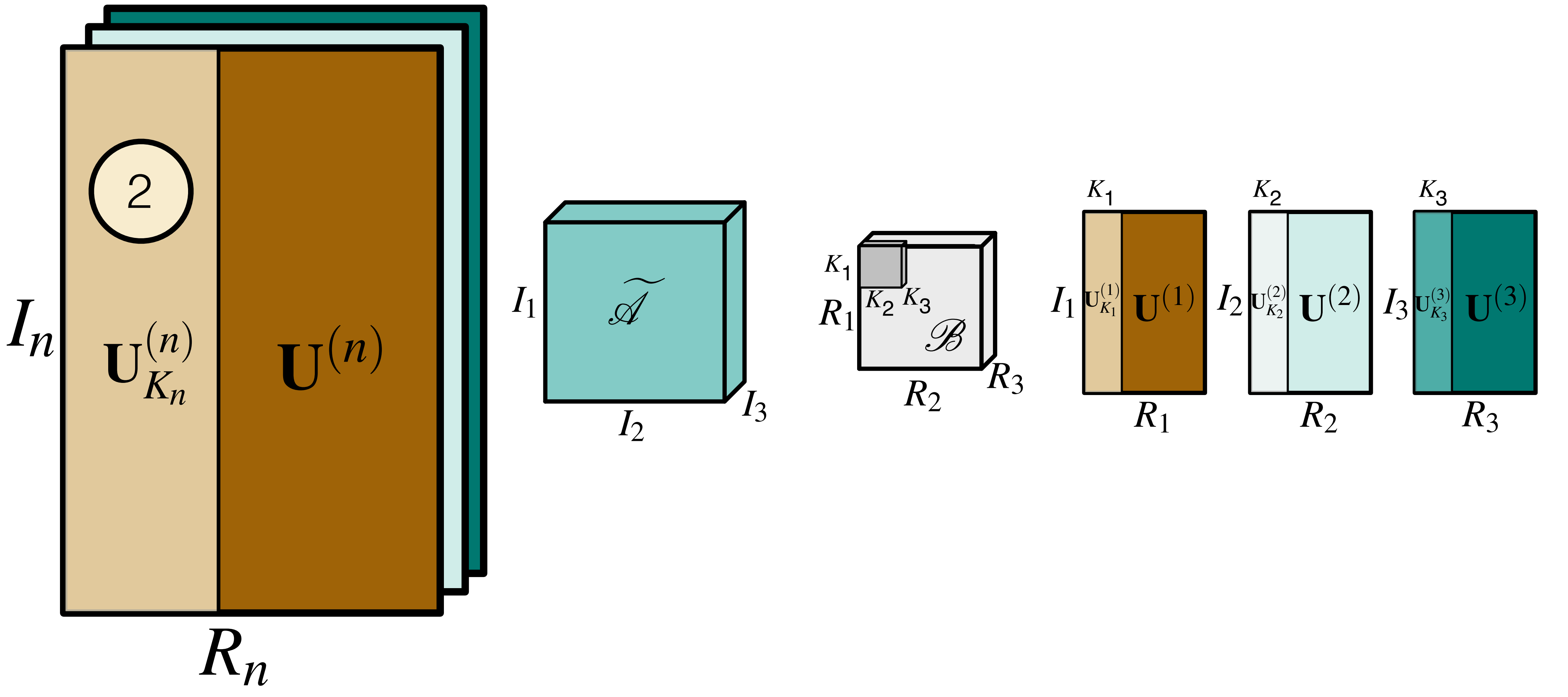
- SVD allows for progressive rank truncation
  - orthogonality of singular vectors
  - order of increasing singular values
- CP does not exhibit good progressive truncation behavior
  - non-orthogonal factor matrices
- All-orthogonal Tucker model supports progressive truncation
  - does not necessarily give best possible progression





Properties of Tucker Factor Matrices

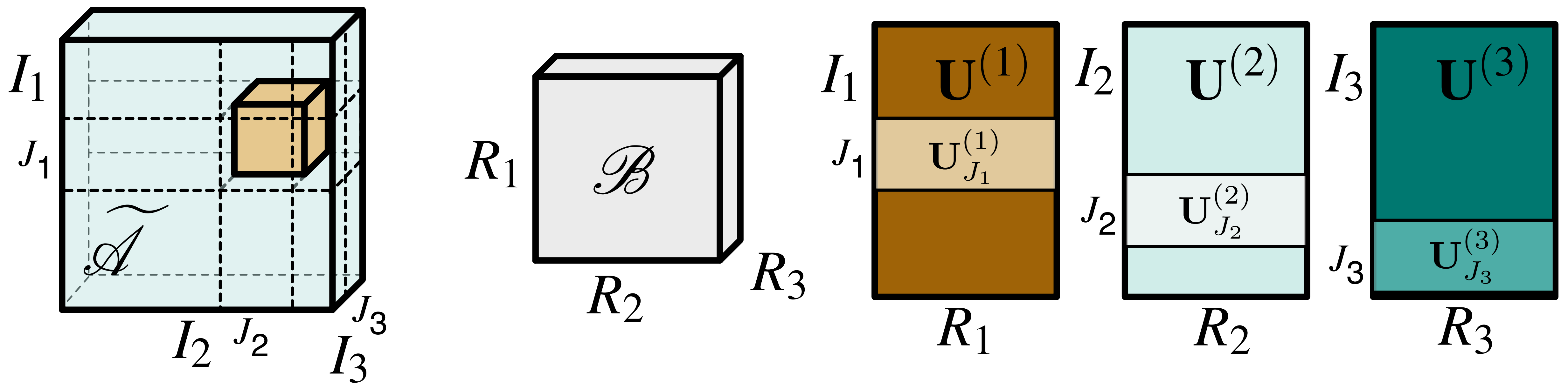




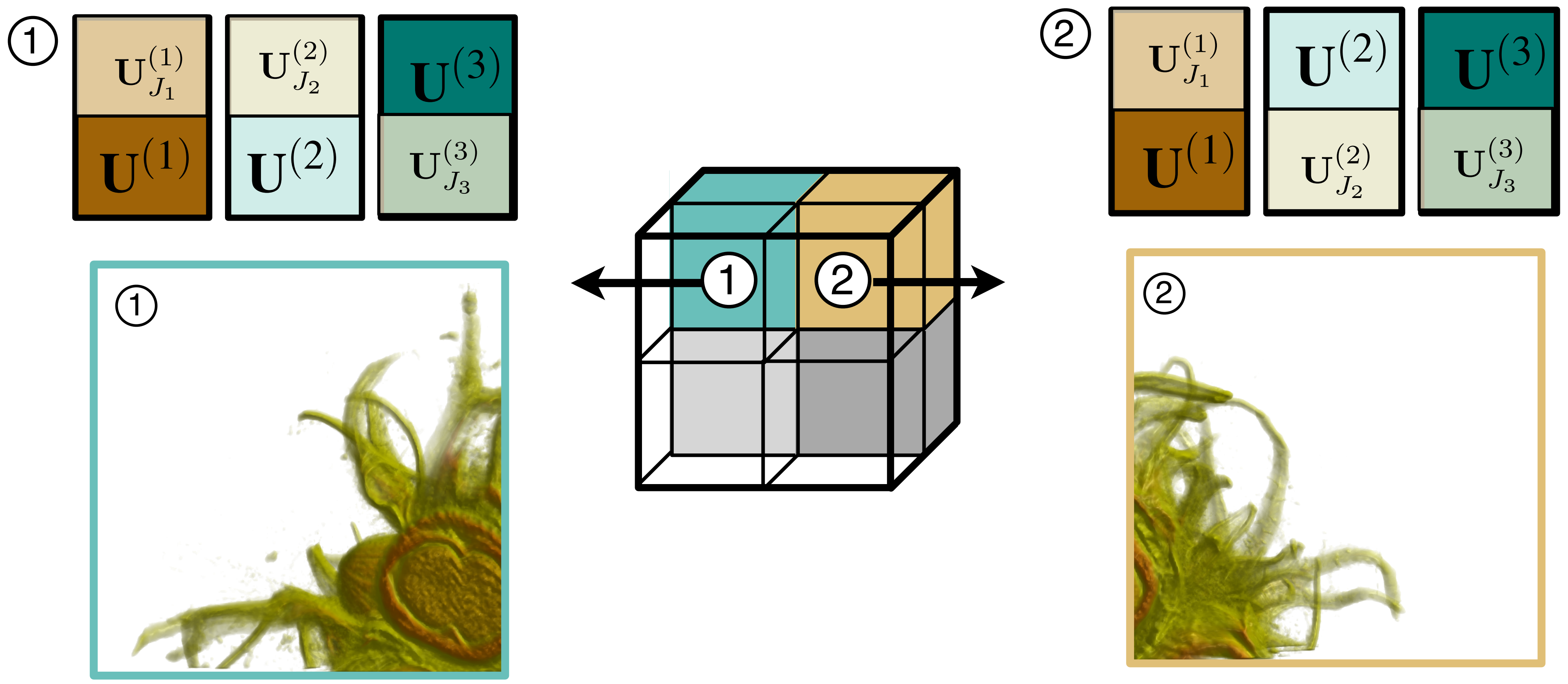
- Vectors along horizontal axis (rows)
  - 1.1; spatial selectivity
  - 1.2; spatial subsampling
- Vectors along vertical axis (columns)
  - 2: rank reduction

Spatial Selection in Factor Matrices

- Select submatrices $\mathbf{U}^{(n)}{}_{J_n}$ (a selection of J_n row vectors)
  - reconstruct only from submatrices and core tensor
- Core tensor stays unchanged
- Potential applications
  - view-frustum culling
  - adaptive spatial selection (multiresolution DVR)

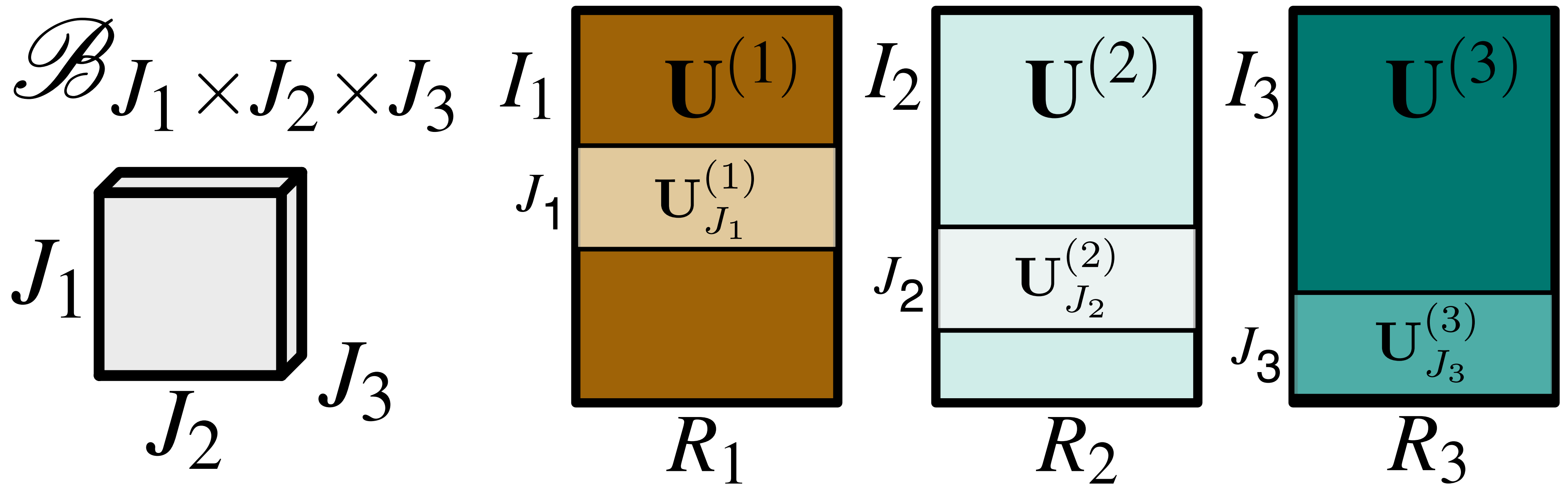


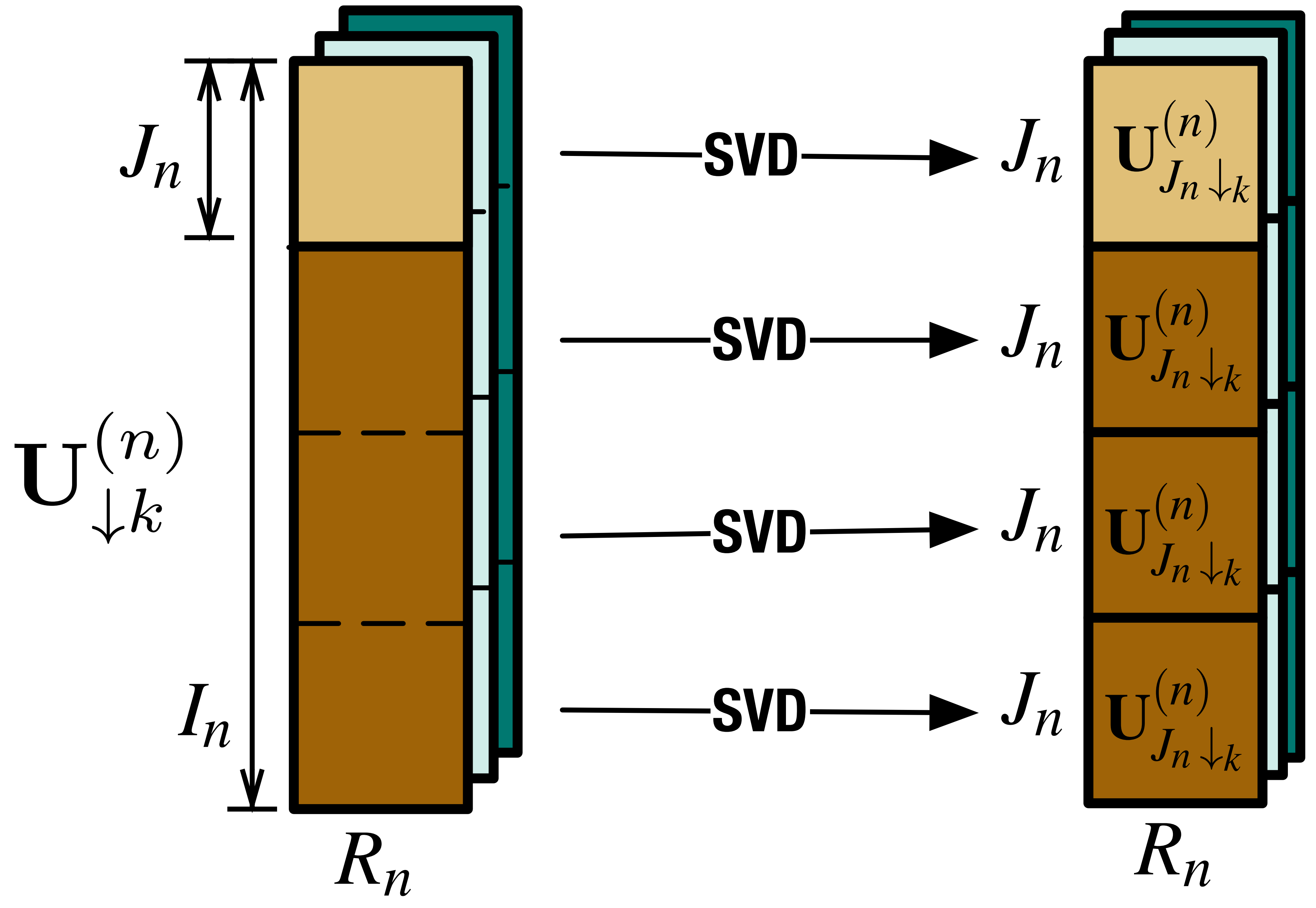
$$\tilde{\mathcal{A}}_{J_1 \times J_2 \times J_3} = \mathcal{B} \times_1 \mathbf{U}^{(1)}_{J_1} \times_2 \mathbf{U}^{(2)}_{J_2} \times_3 \mathbf{U}^{(3)}_{J_3}$$



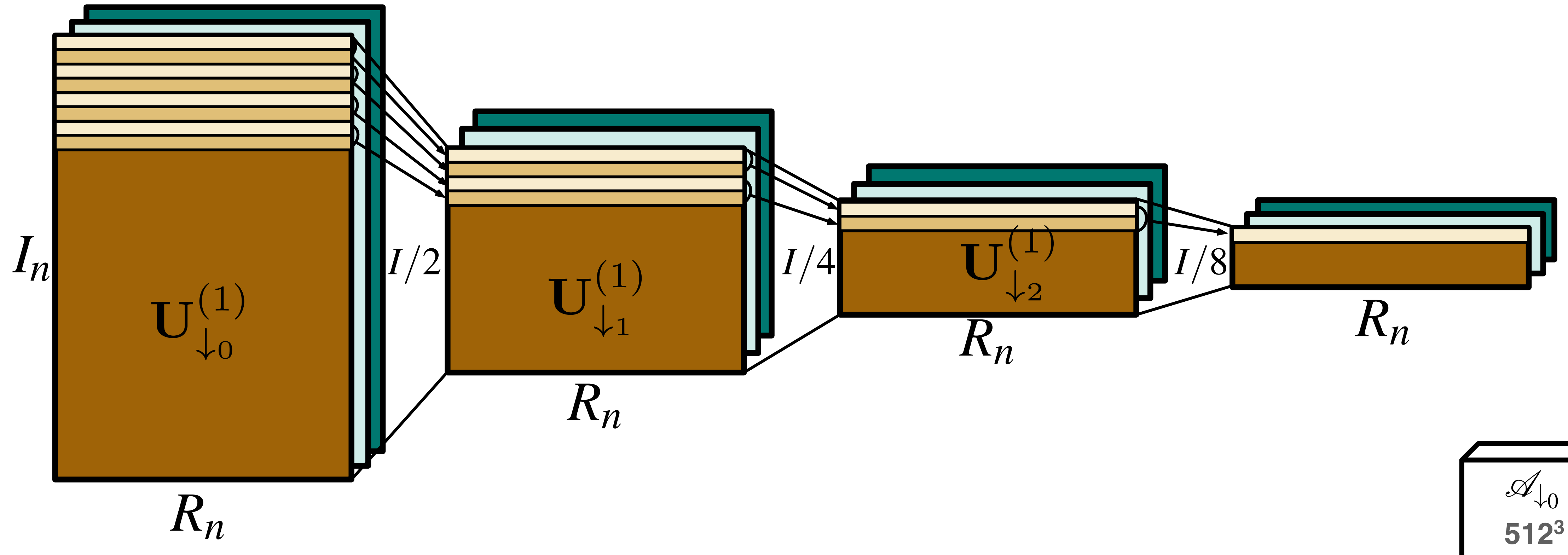
Orthogonality Issues and Truncation

- Spatial selection of factor matrix row ranges destroys the orthogonality property
- Newly derived, spatially local tensor cores from non-orthogonal factor submatrices are not all-orthogonal
  - but only the all-orthogonality makes core tensors rank-reducible
- In order to achieve rank-reducible core tensors, another SVD is applied to spatially selective or averaged submatrices
  - see Tsai and Shih, 2012; Suter, 2013



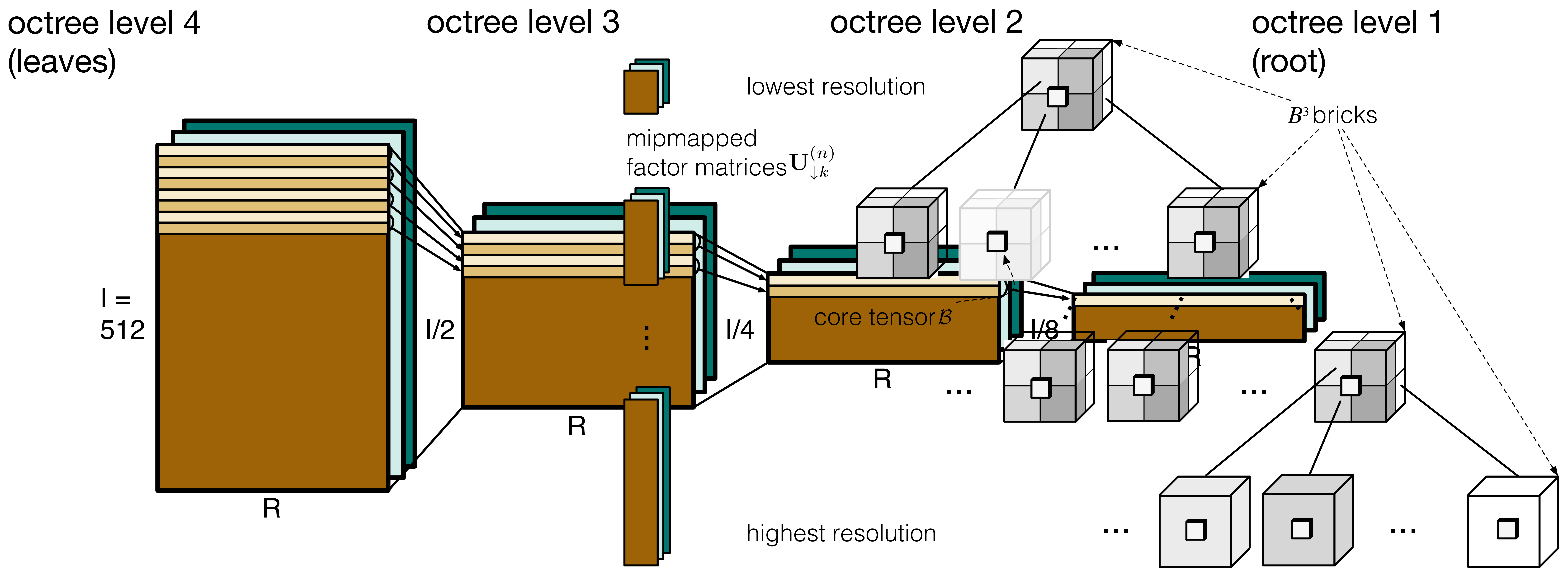


Spatial Subsampling in Factor Matrices

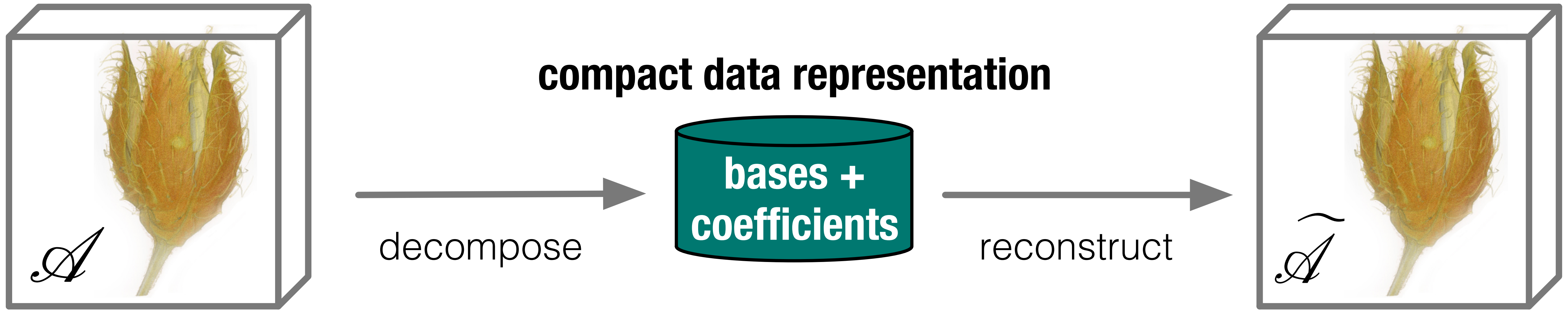


- Spatial correspondence of rows allows for averaging or subsampling of factor matrix row vectors
- Potential applications
  - multiresolution modeling

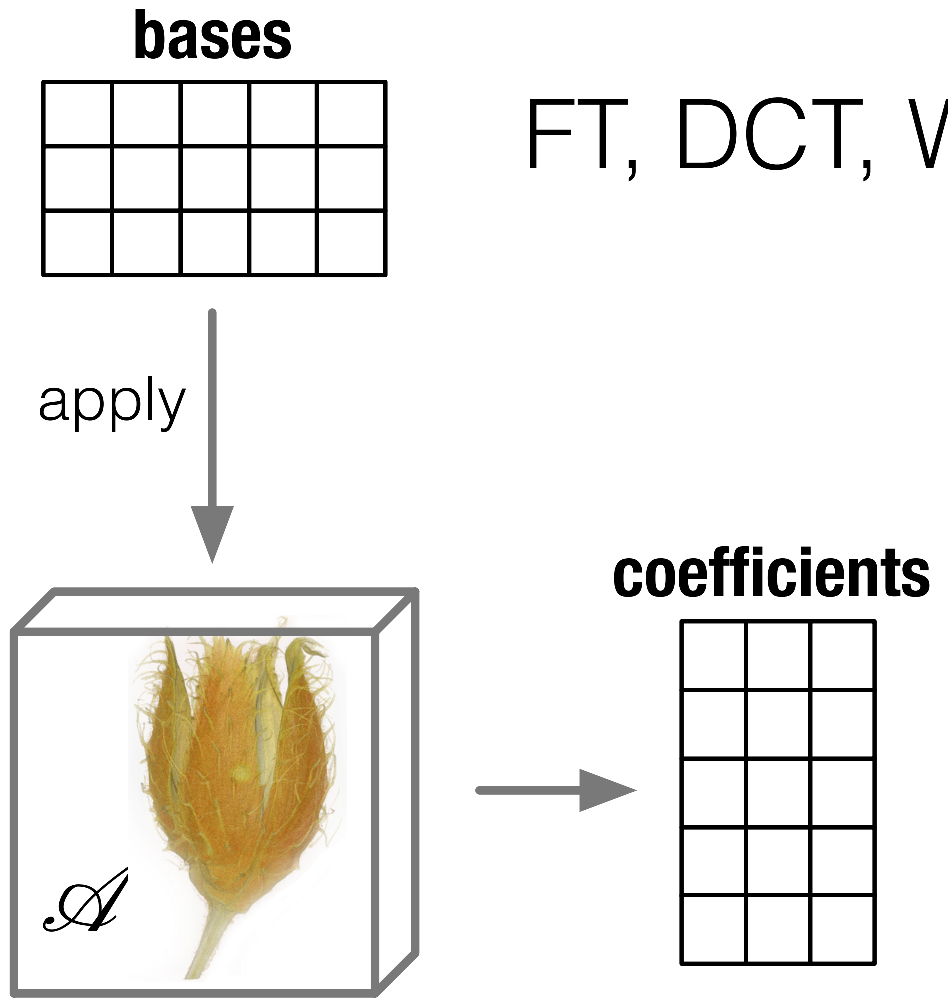
Global Factor Matrices Octree Hierarchy



Pre-Defined vs. Learned Bases

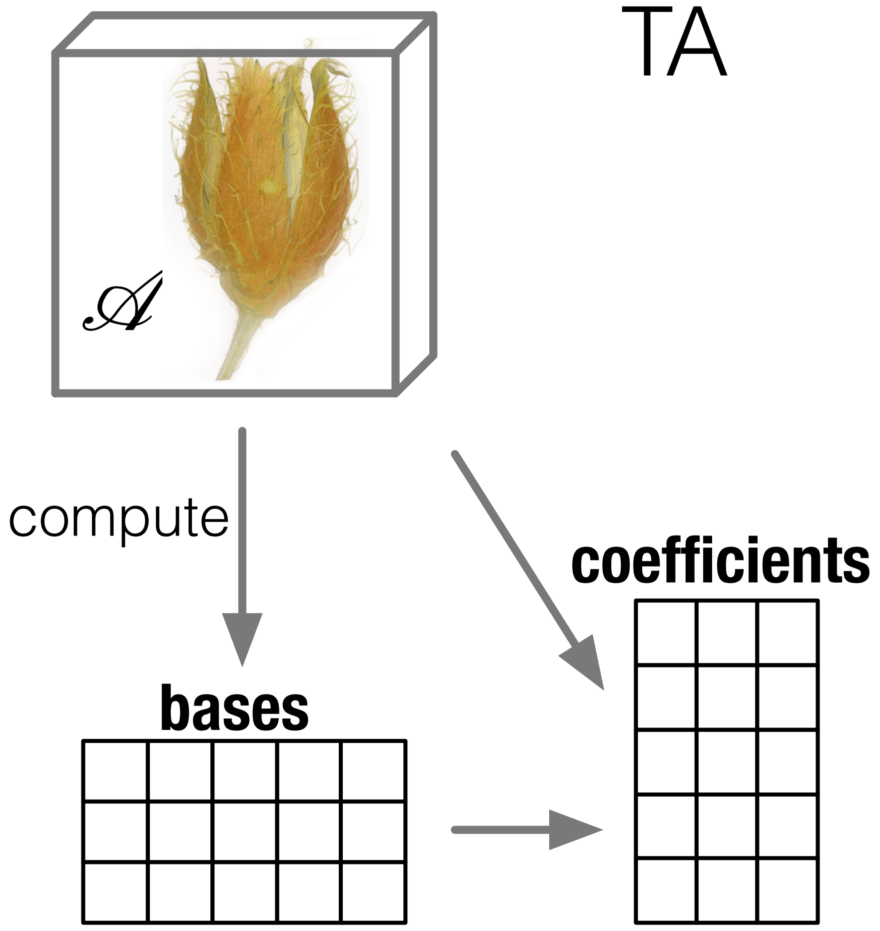


Pre-defined bases



FT, DCT, WT

Learned bases



TA

VISUALIZATIONAND MULTIMEDIALAB

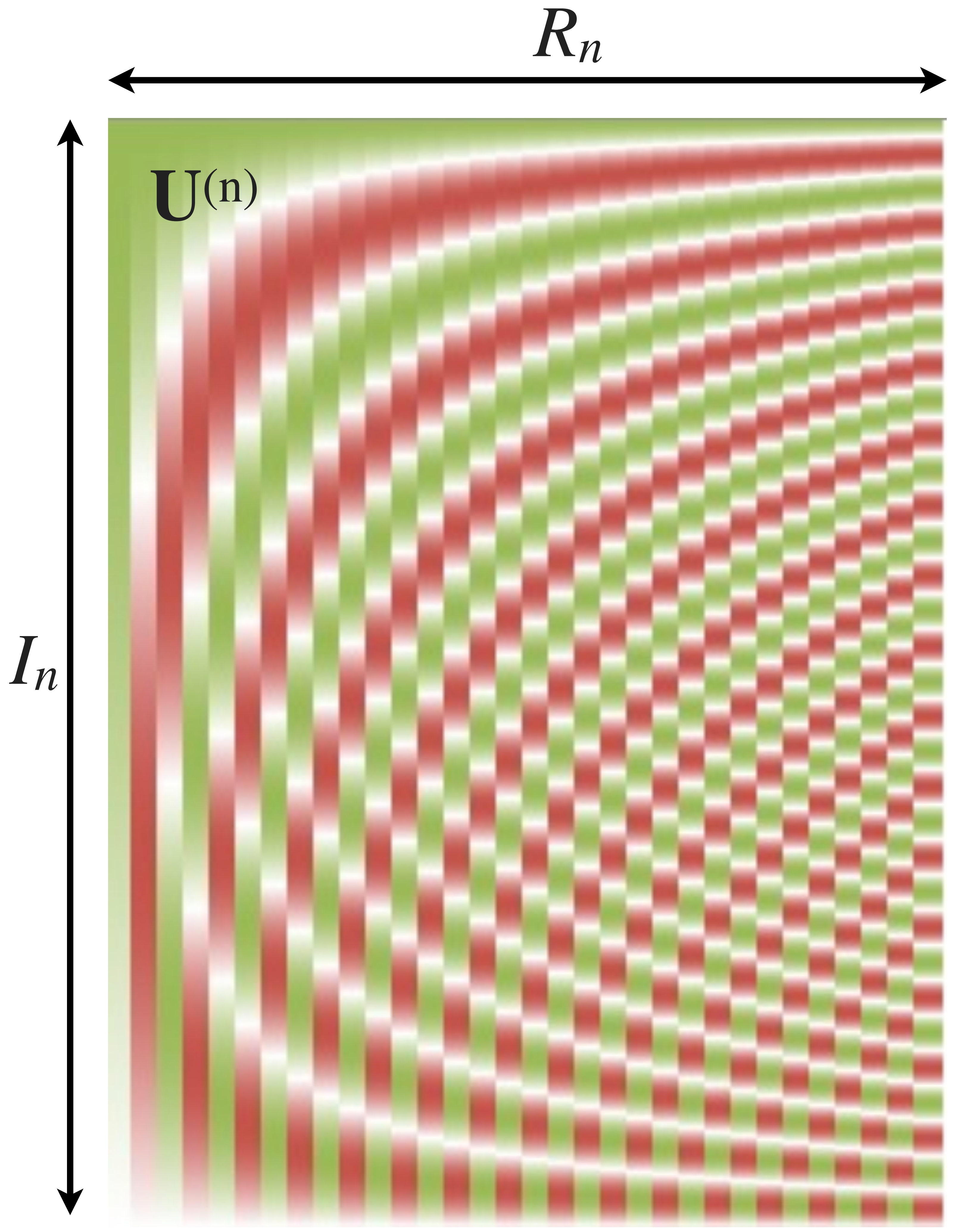
universitätbonn

DCT as Tucker Decomposition

- The DCT of a 2D image or higher order tensor directly maps to the Tucker tensor decomposition model
  - tensor decomposition using pre-defined basis factor matrices
- Using the DCT type-II formulation, the basis matrices $\mathbf{U}^{(n)}$ entries can be formed by:

$$u_{ij}^{(n)} = C_i \cos\left(\frac{(2(j-1)+1)(i-1)\pi}{2I_n}\right)$$

  - where $i \in \{1, \ldots, I_n\}$ and j $\in \{1, \ldots, R_n\}$

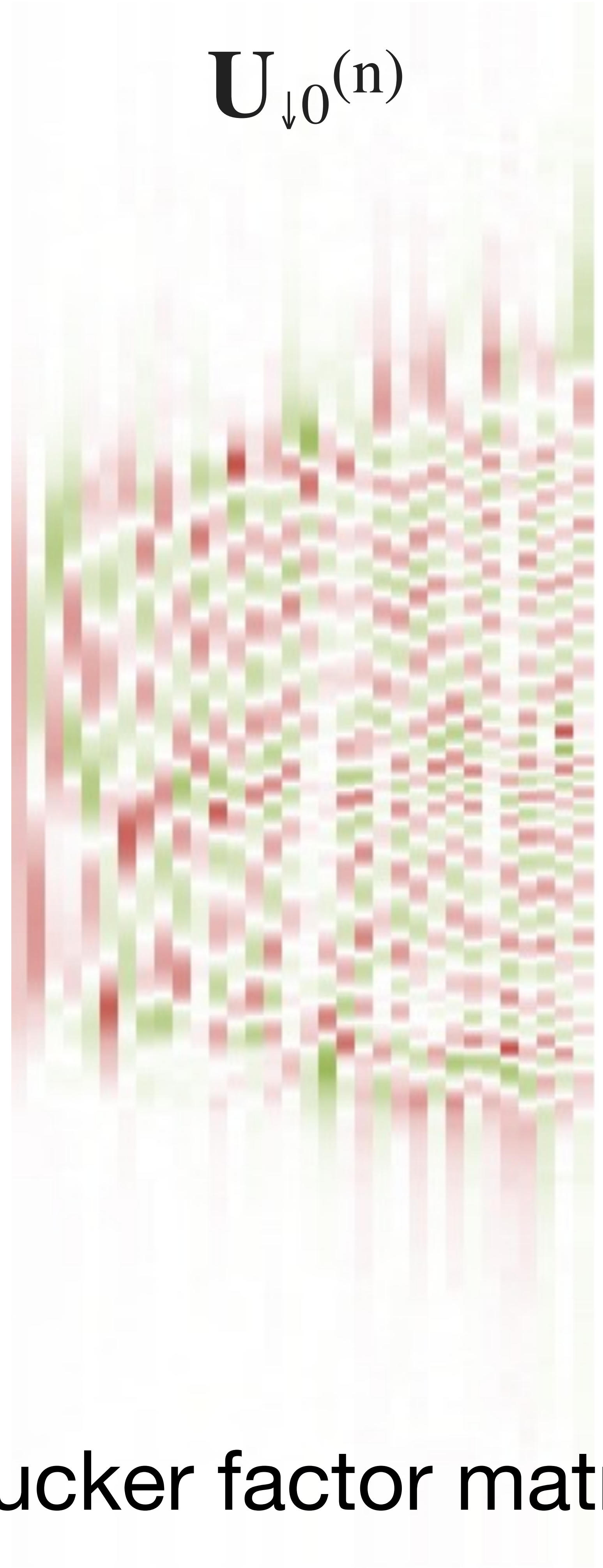


Example of Subsampled TA Factor Matrices

$\mathbf{U}_{\mathbf{DCT}}^{(n)}$

DCT factor matrix

$\mathbf{U}_{\downarrow 0}^{(n)}$



Tucker factor matrices

Tucker Reconstruction

other formulas for CP

$$\widetilde{\mathscr{A}} = \mathscr{B} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)}$$

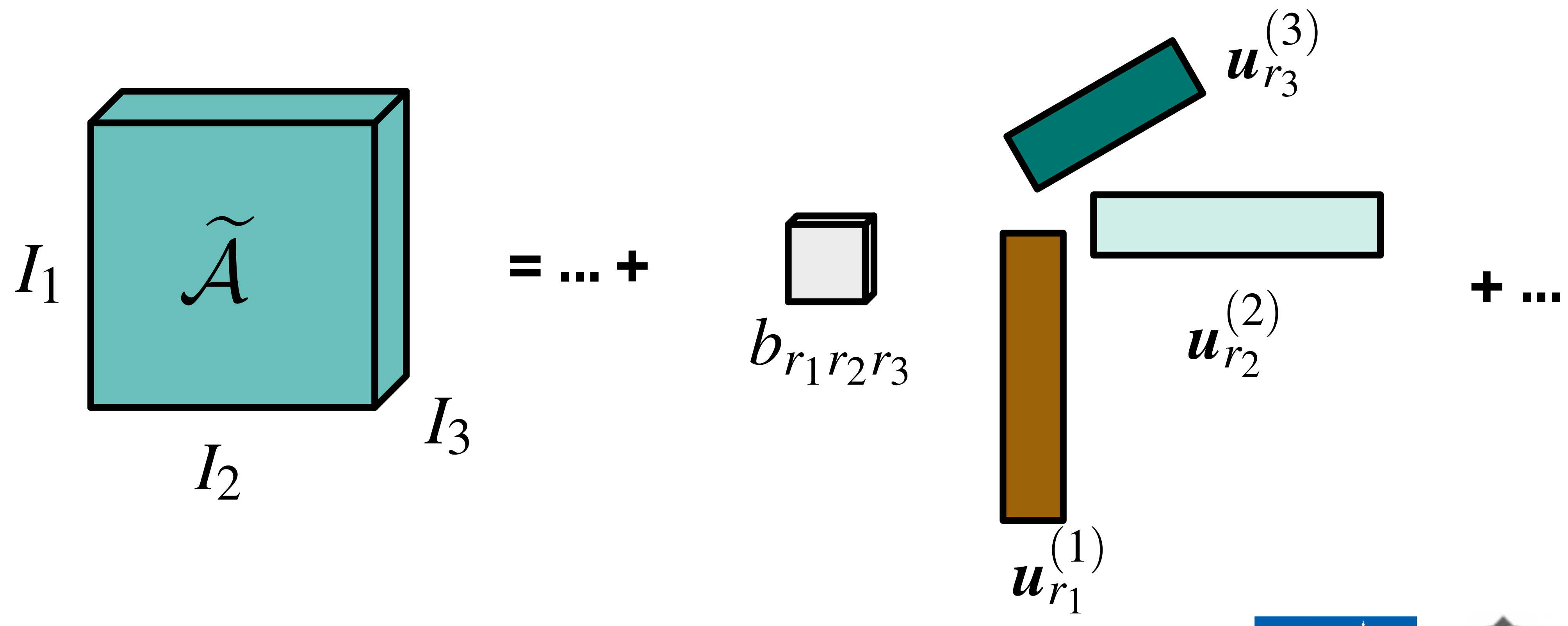
- Reconstruction from rank-one tensors

$$\widetilde{\mathscr{A}} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \sum_{r_3=1}^{R_3} b_{r_1,r_2,r_3} \cdot \boldsymbol{u}_{r_1}^{(1)} \circ \boldsymbol{u}_{r_2}^{(2)} \circ \boldsymbol{u}_{r_3}^{(3)}$$

-> progressive reconstruction

- Element-wise reconstruction

$$\widetilde{a}_{i_1 i_2 i_3} = \sum_{r_1} \sum_{r_2} \sum_{r_3} b_{r_1 r_2 r_3} \cdot u_{i_1 r_1}^{(1)} \cdot u_{i_2 r_2}^{(2)} \cdot u_{i_3 r_3}^{(3)}$$



Reconstruction Complexity

(1)

$$\widetilde{\mathcal{A}} = \sum_{r_k} \mathcal{B}[r_1, \ldots, r_N] \cdot \mathbf{U}^{(1)}_{(r_1)} \otimes \mathbf{U}^{(2)}_{(r_2)} \cdots \otimes \mathbf{U}^{(N)}_{(r_N)}$$

$$\mathrm{O}(R_1 \cdot R_2 \cdot R_3 \cdot I_1 \cdot I_2 \cdot I_3)$$

(2)

$$\widetilde{\mathcal{A}} = \sum_{r} \mathbf{U}^{(1)}_{(r)} \otimes \sum_{s} \mathbf{U}^{(2)}_{(s)} \otimes \sum_{t} \mathcal{B}[r, s, t] \cdot \mathbf{U}^{(3)}_{(t)}$$

$$\mathrm{O}(R_1 \cdot I_1 \cdot I_2 \cdot I_3)$$