CSE 392: Matrix and Tensor Algorithms for Data

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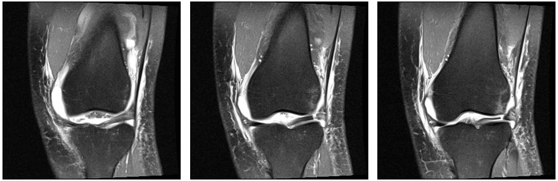
Lecture 15: Introduction to tensors, tensor-matrix products.

Outline

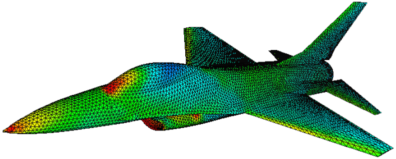
Introduction - A Multi-Dimensional World

- Much of real-world **data** is inherently **multidimensional**

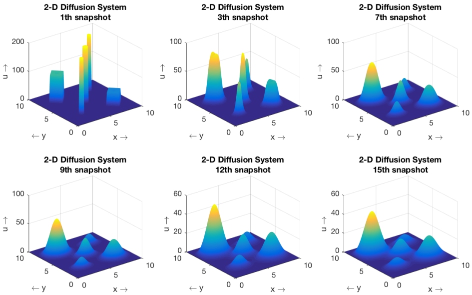

- and is easily stored in/accessed through **high dimensional** arrays



- Many **operators** and **models** are natively **multi-way**



- Simulated data (i.e. intermediate **solutions** can be), too

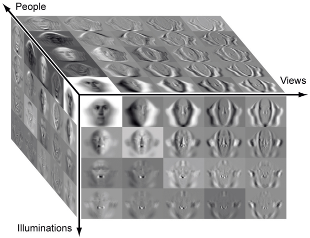


Motivation

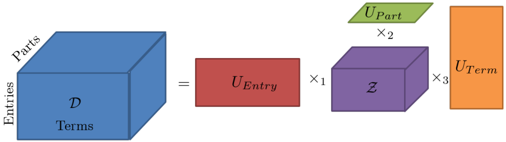
Tensor decompositions give us a way to analyze, compress, and otherwise manipulate operators and data that are far more useful/natural than "flattening" this multidimensional structure into a matrix and using matrix tools.

Tensor Applications

- **Machine vision**: understanding the world in 3D, enable understanding phenomena such as perspective, occlusions, illumination



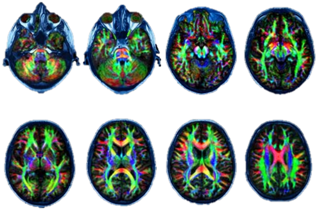
- **Latent semantic tensor indexing**: common terms vs. entries vs. parts, co-occurrence of terms



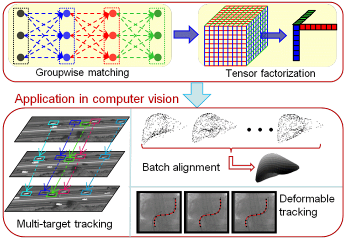
Tensor subspace Analysis for Viewpoint Recognition, Ivanov, Mathies, Vasilescu, ICCV, 2009

Tensor Applications

- **Medical imaging**: naturally involves 3D (spatio) and 4D (spatio-temporal) correlations



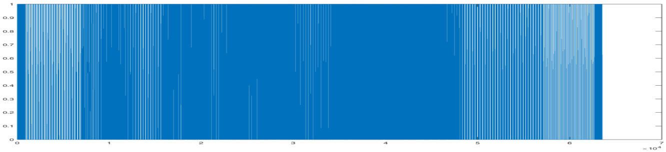
- **Video surveillance and motion signature**: 2D images + 3^{rd} dimension of time, 3D/4D motion trajectory



Shi, Ling, Hu, Yuan, Xing, **Multi-target tracking with motion context in tensor power iteration**, CVPR, 2014

The Power of Representation

- Traditional **matrix-based** methods assuming data **vectorization** are generally **agnostic** to possible **high dimensional correlations**
- What is that ?



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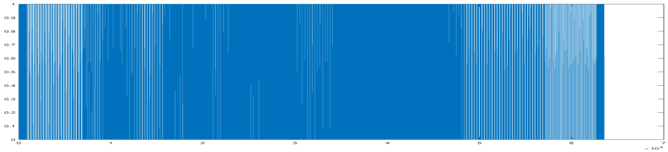

- Observe the same data but in a different (matrix rather than vector) representation

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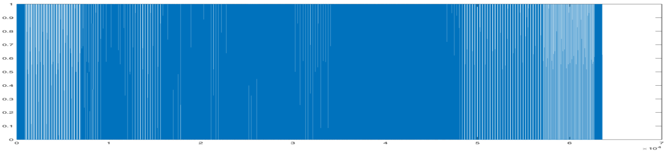

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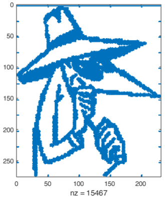


- **Representation matters!** some correlations can only be realized in appropriate representation

Notation and Definition

Uppercase Script: $\mathcal{A}$, is a 3rd order tensor.

Uppercase Bold: $\boldsymbol{X}$, is a matrix.

Bold lowercase: $\boldsymbol{y}$, is a vector OR a $1 \times 1 \times n$ tensor.

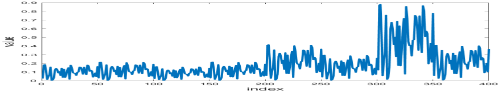
Kronecker Product of an $m \times m$ with an $n \times n$:

$$\boldsymbol{A} := \boldsymbol{G} \otimes \boldsymbol{B} = \begin{bmatrix} g_{11}\boldsymbol{B} & g_{12}\boldsymbol{B} & \cdots & g_{1m}\boldsymbol{B} \\ g_{21}\boldsymbol{B} & \cdots & \cdots & g_{2m}\boldsymbol{B} \\ \vdots & \vdots & \vdots & \vdots \\ g_{m1}\boldsymbol{B} & \cdots & g_{m(m-1)}\boldsymbol{B} & g_{mm}\boldsymbol{B} \end{bmatrix}$$

Kronecker Products synonymous with notion of separability, computational and storage efficiency. These come up a lot in tensor decompositions.

Data Organization Reveals Latent Structure

Suppose $\boldsymbol{y} \in \mathbb{R}^{mn}$



Reshape as $m \times n$ matrix,

$$\mathbf{Y} = \mathbf{u}\mathbf{v}^\top = \mathbf{u} \circ \mathbf{v}$$

$$\Rightarrow \mathbf{y} = \mathbf{v} \otimes \mathbf{u} = \begin{bmatrix} v_1 \boldsymbol{u} \\ v_2 \boldsymbol{u} \\ \vdots \\ v_n \boldsymbol{u} \end{bmatrix}$$

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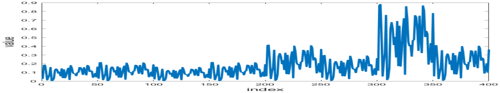

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Implies storage is reduced from mn to $m + n$ numbers, reveals only 1 important direction.

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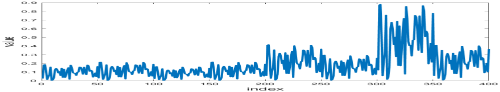

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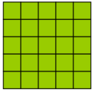
Retaining the higher dimensional format reveals latent structure.

Tensors

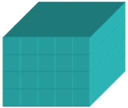
- **Notation** : $\mathcal{A}^{n_1 \times n_2 \ldots, \times n_d}$ - d^{th} order tensor
  - 0^{th} order tensor - **scalar**

  - 1^{st} **order tensor - vector**

  - 2^{nd} **order tensor - matrix**



  - 3^{rd} **order tensor ...**



Tensor Inner Product and Norm

Inner product:

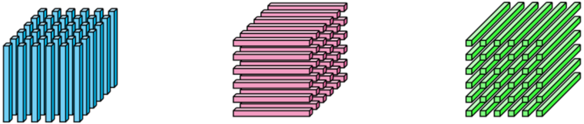
$$\langle \mathcal{A}, \mathcal{B} \rangle = \sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} a_{i_1,\ldots,i_d} b_{i_1,\ldots,i_d}$$

Norm: Unless otherwise specified, norm refers to the Frobenius norm, which in d-dimensional tensorial setting takes the form:

$$\|\mathcal{A}\| = \sqrt{\sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} |a_{i_1,\ldots,i_d}|^2}$$

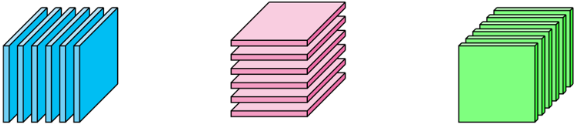
Inside the Box

- *Fiber* - a vector defined by fixing all but one index while varying the rest



mode-1 $\mathcal{A}_{:,j,k}$ | mode-2 $\mathcal{A}_{i,:,k}$ | mode-3 $\mathcal{A}_{i,j,:}$, $\boldsymbol{a}_{ij}$

- *Slice* - a matrix defined by fixing all but two indices while varying the rest



lateral $\mathcal{A}_{:,j,:}$, $\vec{\mathcal{A}}_j$ | horizontal $\mathcal{A}_{i,:,:}$ | frontal $\mathcal{A}_{:,:,k}$, $\boldsymbol{A}^{(k)}$

Accessing Entries

Let $\mathcal{A}$ be the $4 \times 3 \times 2$ tensor with

$$\mathcal{A}_{:,:,1} = \begin{bmatrix} 5 & -1 & 0 \\ 0 & 2 & -1 \\ -3 & 8 & -2 \\ 1 & 4 & .25 \end{bmatrix} \text{ and } \mathcal{A}_{:,:,2} = \begin{bmatrix} .5 & -2 & 0 \\ 6 & -5 & -1 \\ 7 & .5 & 3 \\ 1 & 0 & 1 \end{bmatrix}$$

Exercise: Find

- $\mathcal{A}_{4,:,2}$
- $\mathcal{A}_{2,:,:}$
- $\mathcal{A}_{2,3,:}$
- $\|\mathcal{A}\|^2$

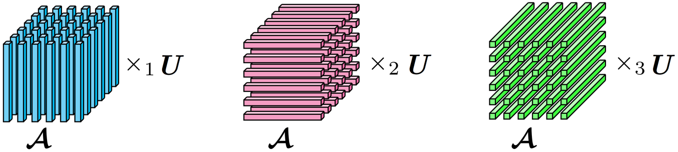
Tensor-Matrix Multiplication

Definition

- The k - mode multiplication of a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ with a matrix $U \in \mathbb{R}^{j \times n_k}$ is denoted by $\mathcal{A} \times_k U$ and is of size $n_1 \times \cdots \times n_{k-1} \times j \times n_{k+1} \times \cdots \times n_d$
- Element-wise

$$(\mathcal{A} \times_k U)_{i_1 \cdots i_{k-1} j i_{k+1} \cdots i_d} = \sum_{i_k=1}^{n_k} a_{i_1 i_2 \cdots i_d} u_{j i_k}$$

- Which view: k-mode multiplication



Matricization makes this concrete...

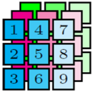
Unfolding - Matricization

A tensor "matricization" refers to (specific) mappings of the tensor to a matrix. Given $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$, the mth mode unfolding maps $\mathcal{A}$ to $\boldsymbol{A}$ via $(i_1, \ldots, i_d) \to (i_m, j)$, and

$$j = 1 + \sum_{k=1, k \neq m}^{d} (i_k - 1) \left(\prod_{l=1, l \neq m}^{k-1} n_l \right).$$

A graphical illustration is more illuminating...

Unfolding - Matricization



(a) Original $\mathcal{A}$.

(b) Mode-1 unfolding $\mathcal{A}_{(1)}$.

(c) Mode-2 unfolding $\mathcal{A}_{(2)}$.

(d) Mode-3 unfolding $\mathcal{A}_{(3)}$.

Graphics: Elizabeth Newman, Tufts Mathematics Ph.D. Thesis, “A Step in the Right Dimension”, 2019

Unfold Example

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Exercise: Find the dimensions of the mode-1, mode-2 and mode-3 unfoldings.

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Mode 1: $4 \times (3 \cdot 2)$

Unfold Example

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Mode 2: $3 \times (2 \cdot 4)$

Unfold Example

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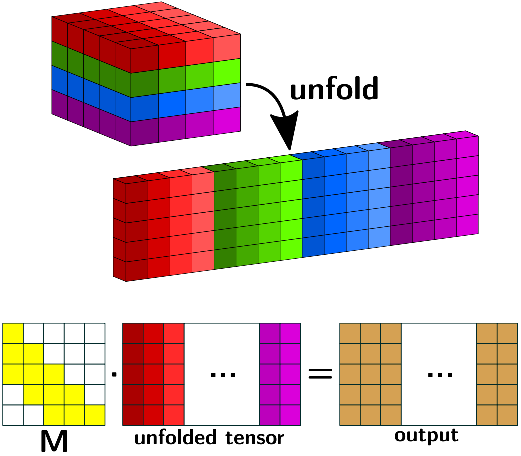
Exercise: Find the dimensions of the mode-1, mode-2 and mode-3 unfoldings.

Mode 3: Put the transposes of the lateral slices side by side, $2 \times (4 \cdot 3)$

k-Mode Product



Tensor-Matrix Products

$$\mathcal{C} = \mathcal{A} \times_n \mathbf{X} \longleftrightarrow \mathbf{C}_{(n)} = \mathbf{X}\boldsymbol{A}_{(n)}$$

<u>Example</u>:

$$\mathcal{A}_{:,:,1} = \begin{bmatrix} 1 & 2 \\ 3 & -2 \end{bmatrix}; \qquad \mathcal{A}_{:,:,2} = \begin{bmatrix} -1 & 4 \\ -3 & 0 \end{bmatrix} \text{ and } \boldsymbol{X} = \begin{bmatrix} 1 & -1 \\ 0 & 2 \end{bmatrix}.$$

$\mathcal{A} \times_1 \boldsymbol{X}$:

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$\mathcal{A} \times_1 \boldsymbol{X}$:

Compute the matrix-matrix product

$$\begin{bmatrix} 1 & -1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 & -1 & 4 \\ 3 & -2 & -3 & 0 \end{bmatrix} = \begin{bmatrix} -2 & 4 & 2 & 4 \\ 6 & -4 & -6 & 0 \end{bmatrix}$$

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$\mathcal{A} \times_1 \boldsymbol{X}$:

Soln: $\mathcal{C}_{:,:,1} = \begin{bmatrix} -2 & 4 \\ 6 & -4 \end{bmatrix}, \qquad \mathcal{C}_{:,:,2} = \begin{bmatrix} 2 & 4 \\ -6 & 0 \end{bmatrix}$

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Class Exercise: Find $\mathcal{A} \times_2 \mathbf{Y}$. (In particular, which mode(dim) expands ?)

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Soln: Form $\mathbf{Y}\boldsymbol{A}_{(2)} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 3 & -1 & -3 \\ 2 & -2 & 4 & 0 \end{bmatrix}$

Tensor-Matrix Products

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Soln: Result is $\begin{bmatrix} 1 & 3 & -1 & -3 \\ 2 & -2 & 4 & 0 \\ 3 & 1 & 3 & -3 \end{bmatrix}$

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Soln: Reshape to get $\mathcal{C}_{:,:,1} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & -2 & 1 \end{bmatrix}, \qquad \mathcal{C}_{:,:,2} = \begin{bmatrix} -1 & 4 & 3 \\ -3 & 0 & -3 \end{bmatrix}$

Tensor-Matrix Products – Contractions

Some tensor-matrix products result in **contraction** of a dimension.

Example: Let $\mathcal{A}$ be size $5 \times 6 \times 7$, and compute $\mathcal{C} := \mathcal{A} \times_3 \mathbf{X}$ where $\mathbf{X}$ is size 2×7.

Solution:

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Solution: Form $\mathbf{X}\mathcal{A}_{(3)}$, which is a 2×7 with a $7 \times (5 \cdot 6)$.

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Solution: Form $\mathbf{X}\mathcal{A}_{(3)}$, which is a 2×7 with a $7 \times (5 \cdot 6)$.
Result is a $2 \times (5 \cdot 6)$ matrix. $\Rightarrow \mathcal{C}$ has dimensions $5 \times 6 \times 2$.

Exercises

$$\mathcal{A}_{:,:,1} = \begin{bmatrix} 5 & -1 & 0 \\ 0 & 2 & -1 \\ -3 & 8 & -2 \\ 1 & 4 & .25 \end{bmatrix} \text{ and } \mathcal{A}_{:,:,2} = \begin{bmatrix} .5 & -2 & 0 \\ 6 & -5 & -1 \\ 7 & .5 & 3 \\ 1 & 0 & 1 \end{bmatrix}$$

Find

- $\mathcal{A} \times_2 \begin{bmatrix} 4 & 1 & 0 \end{bmatrix}$
- $\mathcal{A} \times_3 \begin{bmatrix} 1 & 1 \end{bmatrix}$

The Kronecker Connection

Suppose $\mathcal{C}$ be $n_1 \times n_2 \times \cdots n_d$ and define $\mathcal{A} := \mathcal{C} \times_{j=1}^{d} \boldsymbol{X}_j$, where the matrices $\boldsymbol{X}_j$ have n_j columns, respectively.

Then

$$\mathcal{A}_{(j)} = \boldsymbol{X}_j \mathcal{C}_{(j)} \left(\boldsymbol{X}_d^\top \otimes \boldsymbol{X}_{d-1}^\top \otimes \cdots \otimes \boldsymbol{X}_{j+1}^\top \otimes \boldsymbol{X}_{j-1}^\top \otimes \cdots \otimes \boldsymbol{X}_1^\top \right).$$

This makes clear the separability of the mode-wise matrix products. Note that one or more of the $\boldsymbol{X}_j$ could be identity matrices.

Tensor-Matrix Products

$$\mathcal{C} = \mathcal{A} \times_n \mathbf{X} \longleftrightarrow \mathbf{C}_{(n)} = \mathbf{X}\boldsymbol{A}_{(n)}$$

Note that, for example,

$$\mathcal{A} \times_m \mathbf{X} \times_n \mathbf{Y} = \mathcal{A} \times_n \mathbf{Y} \times_m \mathbf{X}.$$

Exercise: Prove the identity above!

Example: Let $\mathcal{A}$ be third order. Then $\widetilde{\mathcal{A}} := \mathcal{A} \times_1 \boldsymbol{X} \times_2 \mathbf{Y} = \mathcal{A} \times_1 \boldsymbol{X} \times_2 \mathbf{Y} \times_3 \mathbf{I}$ can be understood as $\widetilde{\mathcal{A}}_{(1)} = \boldsymbol{X}\mathcal{A}_{(1)}(\mathbf{I} \otimes \mathbf{Y}^\top)$, and folding.

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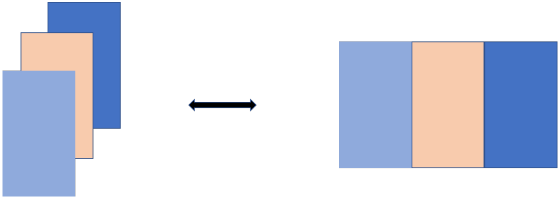

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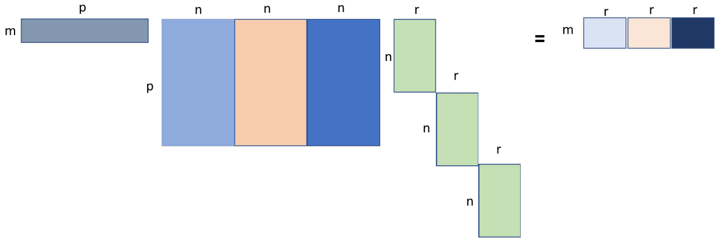
Example: Let $\mathcal{A}$ be third order. Then $\widetilde{\mathcal{A}} := \mathcal{A} \times_1 \boldsymbol{X} \times_2 \mathbf{Y} = \mathcal{A} \times_1 \boldsymbol{X} \times_2 \mathbf{Y} \times_3 \mathbf{I}$



Tensor-Matrix Products

$$\mathcal{C} = \mathcal{A} \times_n \mathbf{X} \longleftrightarrow \mathbf{C}_{(n)} = \mathbf{X}\boldsymbol{A}_{(n)}$$

Note that, for example,

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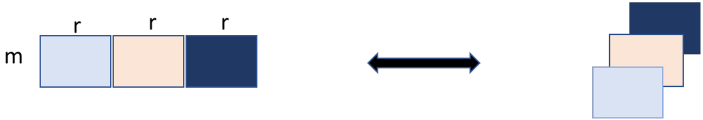

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In particular, implies $\widetilde{\mathcal{A}}_{:,:,i} = \boldsymbol{X}\mathcal{A}_{:,:,i}\mathbf{Y}^\top$; in this example, contracting 2 of the 3 dimensions. So, $\mathcal{A}$ is $p \times n \times 3$, $\tilde{\mathcal{A}}$ is $m \times r \times 3$, where $m < p, n < r$.

Example 2

Let $\mathcal{A} \in \mathbb{R}^{1\times 1\times n}$, that is, just a tube fiber.

Let $\mathbf{M}$ be an $n \times n$ matrix.

Class Exercise: What is the equivalent matrix-arithmetic operation to

$$\mathcal{A} \times_3 \mathbf{M}?$$

Example 3

Let $\mathcal{A} \in \mathbb{R}^{m\times p\times n}$, and let $\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}$ be orthogonal $m \times m, p \times p, n \times n$ matrices, respectively.

Exercise: Show $\|\widehat{\mathcal{A}}\|_F = \|\mathcal{A}\|_F$, where

$$\widehat{\mathcal{A}} = \mathcal{A} \times_1 \boldsymbol{U}^\top \times_2 \boldsymbol{V}^\top \times_3 \boldsymbol{W}^\top.$$

Definition

Recall that $\boldsymbol{P} \in \mathbb{R}^{n \times n}$ is called an orthogonal projection matrix if $\boldsymbol{P}^T = \boldsymbol{P}$ and $\boldsymbol{P}^2 = \boldsymbol{P}$.

Orthogonal projection matrices are not necessarily orthogonal – indeed, they are often not full rank: e.g. if $\mathbf{v}$ has unit length then $\boldsymbol{P} := \mathbf{v}\mathbf{v}^T$ is an orthogonal projector onto $\text{span}\{\mathbf{v}\}$.

Example 4

Let $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$, and let $\mathbf{P}_k, k = 1, 2, 3$ be $n_k \times n_k$ orthogonal projection matrices.

Exercise: Show that for any $k = 1, 2, 3$

$$\|\mathcal{A} - \mathcal{A} \times_k \mathbf{P}_k\|_F = \|\mathcal{A} \times_k (\mathbf{I} - \mathbf{P}_k)\|_F$$

Exercise: Show that $\boldsymbol{P}_k \otimes \mathbf{I}$, $\mathbf{I} \otimes \boldsymbol{P}_k$ are orthogonal projection matrices.

Exercise**: Now show

$$\|\mathcal{A} - \mathcal{A} \times_1 \mathbf{P}_1 \times_2 \boldsymbol{P}_2 \times_3 \boldsymbol{P}_3\|^2 = \|\mathcal{A} \times_1 (\mathbf{I} - \boldsymbol{P}_1)\|^2 + \|\mathcal{A} \times_1 \mathbf{P}_1 \times_2 (\mathbf{I} - \mathbf{P}_2)\|^2 + \|\mathcal{A} \times_1 \mathbf{P}_1 \times_2 \mathbf{P}_2 \times (\mathbf{I} - \mathbf{P}_3)\|^2.$$

Questions?