Higher Order Orthogonal Iteration of Tensors

Multi-Linear Subspace Learning

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- Can be considered as a unified view of dimension reduction techniques
- PCA - a special instance of HOOI

Agenda

- Primer on Principal Component Analysis(PCA), Single Value Decomposition(SVD) and Tensors
- Higher Order Orthogonal Iteration
- Relation of PCA and HOOI
- Application to Dimensionality Reduction

Principal Component Analysis

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  - transformation of data from a high-dimensional space into a low-dimensional space
  - this lower dimensional data - retains meaningful properties of the original data

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- Smaller data sets -
  - easier to explore and visualize
  - makes analyzing data much easier and faster for machine learning algorithms
  - without extraneous variables to process.

PCA (two dimensional idea)

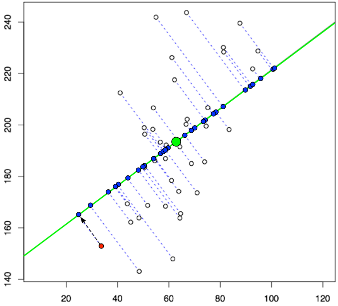

Figure 1: PCA in 2D

PCA (Mathematical Treatment I)

Let us take a model problem. We are given a set of matrices $M_k, k = 1, 2, \ldots K$, all of the same dimension $I \times J$.

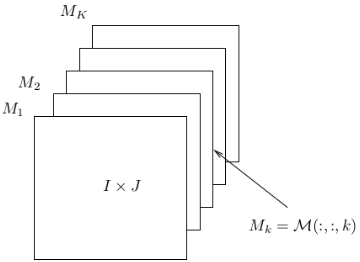

Figure 2: Set of K matrices $M_k R \in I \times J$ represented as an $I \times J \times K$ tensor $\mathcal{M}$

Tensor PCA and HOOI

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- where $A \equiv [y_1, y_2, ...y_K]$, $y_i = x_i - \mu$, $i = 1, .., K$

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- where $U_r = [u_1, ..., u_r]$ and $\Lambda_r = diag\{\lambda_1, ..., \lambda_r\}$
- note that U_r is the orthogonal vector and Λ_r is the diagonal matrix with the diagonal as the eigenvalues.

PCA (Mathematical Treatment IV)

Finally, we reorient the data from the original axes to the ones represented by the principal components. For that we project the original data points x_i to the space of U_r to obtain,

$$\widetilde{x}_i = U_r^T(x_i - \mu)$$

$$x_i = \mu + U_r \widetilde{x}_i$$

PCA and HOOI

SVD

Any real matrix $A_{m\times n}$ can be written (factorized) in the form of a product of three matrices $U_{m\times m}$, $\Sigma_{m\times n}$ and $V^T_{n\times m}$. This process is known as singular value decomposition. The diagonal entries $\sigma_i = \Sigma_{ii}$ of Σ are known as the singular values of M. Mathematically,

$$A = U\Sigma V^T$$

Relevance of SVD in our Discussion

As we discussed in the earlier slides for PCA

- $C = U_r \lambda_r U_r^T$, $\mu = \frac{1}{K}\sum_{i=1}^{K} x_i$, $C = AA^T \in R^{N \times N}$

This U_r can be obtained using SVD also.

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- $$A \approx U_r \Sigma_r V_r^T$$
- where $\Sigma_r = diag\{\sigma_1, ..., \sigma_r\} \in R^{r \times r}$ is the diagonal matrix containing the r largest singular values of A in the descending order $\sigma_1, \sigma_2, ..., \sigma_r$

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- PARFAC, HOSVD utilizes tensors
- Next few slides - some mathematical aspects of Tensor calculations required for HOOI

Tensor Maths I

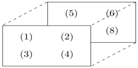
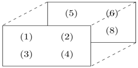


Figure 3: $\mathcal{A}$, a $2 \times 2 \times 2$ matrix



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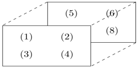

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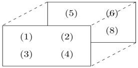

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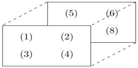

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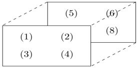

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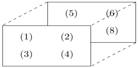

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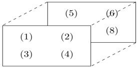

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- $$dist(\mathcal{A}, \mathcal{B}) = \|\mathcal{A} - \mathcal{B}\|_F$$

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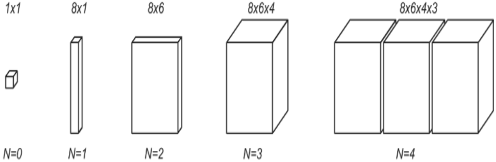

Figure 5: Illustration of tensors of order N= 0,1,2,3,4.

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- Next lets, look at mode-n vectors and mode-n slices of $\mathcal{A}$.

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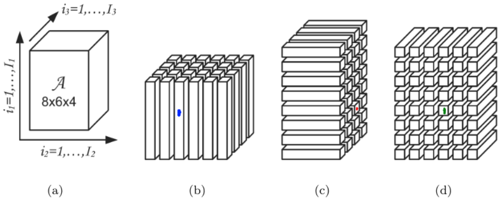

Figure 6: Illustration of the mode-n vectors: (a) a tensor $\mathcal{A} \in \mathbb{R}^{8\times6\times4}$,(b) the mode-1 vectors, (c) the mode-2 vectors, and (d) the mode-3 vectors.

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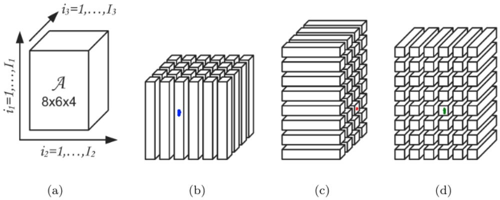
- 

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- notation, blue - $\mathcal{A}(:, 3, 1)$, red - $\mathcal{A}(6, :, 3)$, green - $\mathcal{A}(5, 4, :)$

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- Similarly, the i_nth **mode-n slice** of $\mathcal{A}$ are defined as the $(N-1)$th-order tensor obtained by fixing the mode-n index of $\mathcal{A}$ to be i_n: $\mathcal{A}(:, \ldots :, i_n, :, \ldots, :)$

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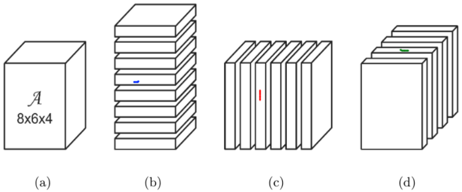

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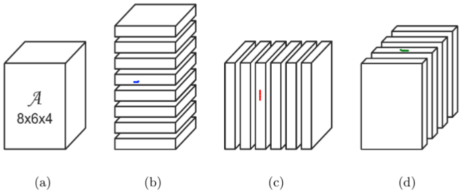
- 

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Tensor Maths IV (Basic Operations - Unfolding)

- Also known as tensor to matrix transformation, flattening, matricization

properties

Tensor Maths IV (Basic Operations - Unfolding)

- Also known as tensor to matrix transformation, flattening, matricization
- A tensor can be unfolded into a matrix by rearranging its **mode-n** vectors.The **mode-n unfolding** of $\mathcal{A}$ is denoted by $A_{(n)} \in \mathbb{R}^{I_n \times (I_1 \times \ldots \times I_n - 1 \times I_n + 1 \times \ldots \times I_N)}$, where the column vectors of $A_{(n)}$ are the **mode-n** vectors of $\mathcal{A}$.

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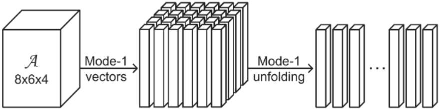

Figure 8: Visual illustration of the mode-1 unfolding from $\mathcal{A}_{8\times6\times4}$ to $A_{8\times24}$

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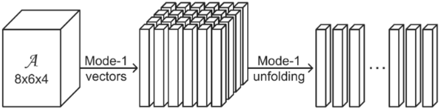
- 

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- Similarly vectorization would provide a 192×1 matrix.

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- where each entry of $\mathcal{B}$ is defined as the sum of products of corresponding entries in $\mathcal{A}$ and U:

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- equivalent to premultiplying each mode-n vector of $\mathcal{A}$ by U. Thus,the mode-n product above can be written using the mode-n unfolding as

$$B_{(n)} = UA_{(n)}$$

Tensor Maths IV (Basic Operations - Mode-*1* product)

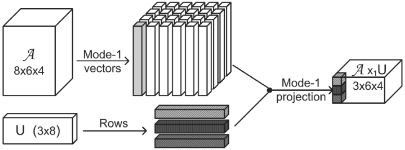

Figure 9: Visual illustration of the mode-n(mode-1) multiplication

Tensor Maths V (Some Properties of Mode Multiplication)

- multiplication of more than mode possible, order immaterial provided the modes are distinct $\mathcal{A} \times_{n_1} U_{n_1} \times_{n_2} U_{n_2} \ldots \times_{n_p} U_{n_p}$

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- optimal $\mathcal{B} = \mathcal{A} \times_{(1)} {U^{(1)}}^T \times_{(2)} {U^{(2)}}^T \ldots \times_T {U^{(T)}}^T$ properties

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- HOOI algo. for 3^{rd} order tensor is explained in the next slide. Extension to higher order tensors is straightforward.

HOOI - Algorithm

input : $\mathcal{A}_{I\times J\times K}$ and r_1, r_2, r_3
output: $L \in \mathbb{R}^{I\times r_1}$, $R \in \mathbb{R}^{I\times r_2}$, $V \in \mathbb{R}^{I\times r_3}, \mathcal{B}$

Choose initial R, V with orthonormal columns ;

while *until convergence* **do**

$\mathcal{C} = \mathcal{A} \times_2 R^T \times_3 V^T$;
$L = SVD(r_1, \mathcal{C}_{(1)})$;
$\mathcal{D} = \mathcal{A} \times_1 L^T \times_3 V^T$;
$R = SVD(r_2, \mathcal{D}_{(2)})$;
$\mathcal{E} = \mathcal{A} \times_1 L^T \times_2 R^T$;
$V = SVD(r_3, \mathcal{E}_{(3)})$;

end

$\mathcal{B} = \mathcal{E} \times_3 V^T$

Algorithm 1: HOOI

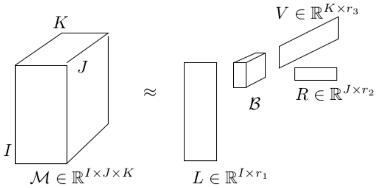

Figure 10: $\mathcal{M}$ approximated by $\mathcal{B} \times_1 L \times_2 R \times_3 V$. $\mathcal{B}$- core tensor, $L(U^{(1)}), R(U^{(2)}), V(U^{(3)})$ are projection matrices

Relation between PCA and HOOI

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  - using PCA to compute projection matrix $U_r \in \mathbb{R}^{IJ \times r}$

PCA Review

1. Introduction
2. Primer
3. HOOI
4. PCA and HOOI
5. Application of HOOI
6. References

Application

- HOOI is useful for dimension reduction because the memory required to store projection matrices L, R, and V and the core tensor $\mathcal{B}$, i. e., $Ir1 + Jr2 + Kr3 + r1r2r3$ is often significantly less than the storage IJK required for the original $I \times J \times K$ tensor, $\mathcal{M}$.

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- Can be used in classification as well as regression tasks dimensionality reduction

[1] Bernard N. Sheehan and Yousef Saad *Higher order orthogonal iteration of tensors (HOOI) and its relation to PCA and GLRAM.*. Proceedings of the 2007 SIAM International Conference on Data Mining. Society for Industrial and Applied Mathematics, 2007.

[2] Haiping Lu *Multilinear Subspace Learning: Dimensionality Reduction of Multidimensional Data*. CRC Press, 2012.

Thanks!