Tensor decomposition

Jean Kossaifi

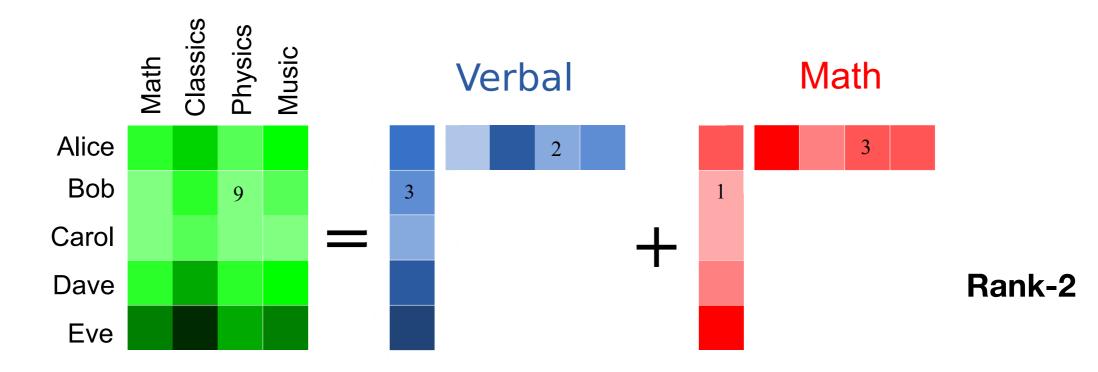


Example: factor analysis

- Spearman worked on understanding whether intelligence is a composite of measurable intelligences
- Intelligence = quantitative and verbal ?
- Score matrix of n students x m subjects

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Matrix decomposition

$$\mathbf{X} \in \mathbb{R}^{m,n}$$

$$\mathbf{X} = \mathbf{AB}, \quad \mathbf{A} \in \mathbb{R}^{m,p+1}, \mathbf{B} \in \mathbb{R}^{p+1,n}, p+1 \le min(m,n)$$

$$\mathbf{A}\mathbf{B} = \sum_{k=0}^{p} \mathbf{a}_{:,k} \mathbf{b}_{k,:}^{\mathsf{T}} = \sum_{k=0}^{p} \mathbf{a}_{:,k} \circ \mathbf{b}_{k,:}$$
rank-1 components

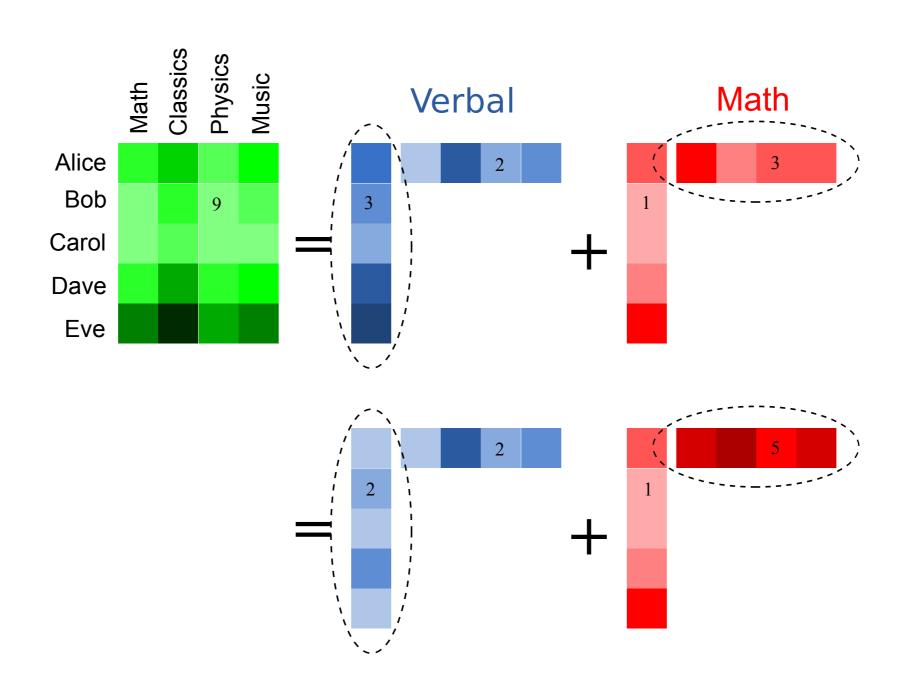
$$\mathbf{C} = \begin{pmatrix} a_{0,0} \\ a_{1,0} \\ \vdots \\ a_{m,0} \end{pmatrix} \begin{pmatrix} a_{0,0}b_{0,0} & a_{0,0}b_{0,1} & \cdots & a_{0,0}b_{0,n} \\ a_{1,0}b_{0,0} & a_{1,0}b_{0,1} & \cdots & a_{1,0}b_{0,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,0}b_{0,0} & a_{m,0}b_{0,1} & \cdots & a_{m,0}b_{0,n} \end{pmatrix} + \cdots + \begin{pmatrix} a_{0,p} \\ a_{1,p} \\ \vdots \\ a_{m,p} \end{pmatrix} \begin{pmatrix} a_{0,p}b_{p,0} & a_{0,p}b_{p,1} & \cdots & a_{0,p}b_{p,n} \\ a_{1,p}b_{p,0} & a_{1,p}b_{p,1} & \cdots & a_{1,p}b_{p,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,p}b_{p,0} & a_{m,p}b_{p,1} & \cdots & a_{m,p}b_{p,n} \end{pmatrix}$$

Ambiguity of Matrix Decomposition

• Low rank decomposition of matrix: $\mathbf{M} = \sum_{k=0}^{K-1} \mathbf{a}_k \mathbf{b}_k^{\mathsf{T}} = \mathbf{A} \mathbf{B}^{\mathsf{T}}$

• One possible choice (SVD on M): $\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathsf{T}}$ $\mathbf{A} = \mathbf{U}\mathbf{S}$ $\mathbf{B} = \mathbf{V}^{\mathsf{T}}$

Ambiguity of Matrix Decomposition



Ambiguity of Matrix Decomposition

• Low rank decomposition of matrix: $\mathbf{M} = \sum_{k=0}^{N-1} \mathbf{a}_k \mathbf{b}_k^{\mathsf{T}} = \mathbf{A} \mathbf{B}^{\mathsf{T}}$

• One possible choice (truncated SVD on M): $\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathsf{T}}$

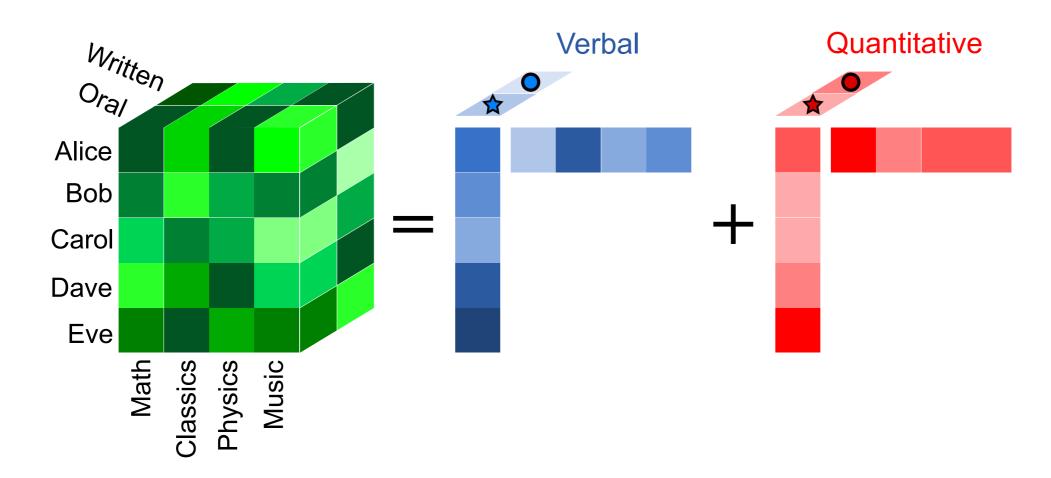
$$A = U[:, :R]S[:R, :R]$$
 $B = V^{T}[:R., :]$

• For any orthonormal matrix $\mathbf{R} \in \mathbb{R}^{R \times R}$ such that $\mathbf{R}\mathbf{R}^{\top} = \mathbf{R}^{\top}\mathbf{R} = \mathbf{I}_{R}$

$$\mathbf{M} = \mathbf{A} \mathbf{R} \mathbf{R}^{\mathsf{T}} \mathbf{B}^{\mathsf{T}} = (\mathbf{A} \mathbf{R}) (\mathbf{R} \mathbf{B})^{\mathsf{T}}$$

From matrix to tensor

- Imagine exam having two parts: written and oral
 -> 2 score matrices (frontal slices of a n*m*2 tensor)
- Verbal skills might matter more in oral exams

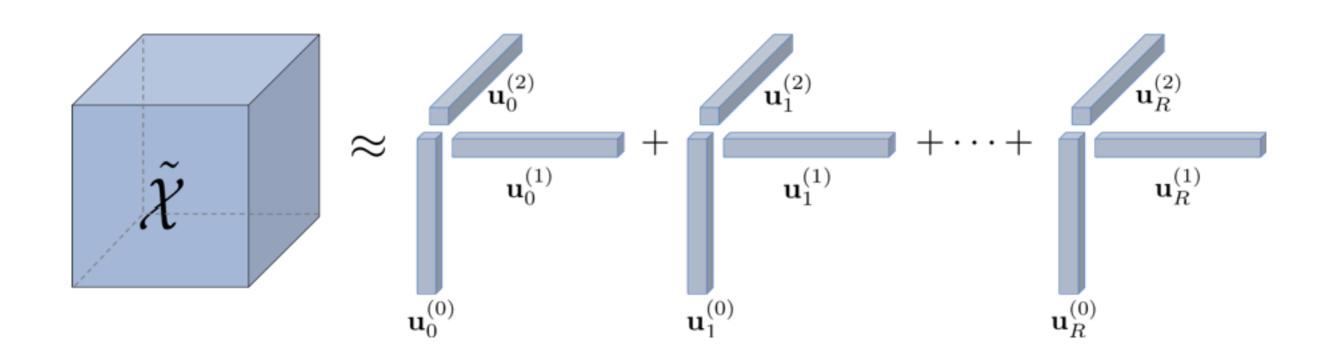


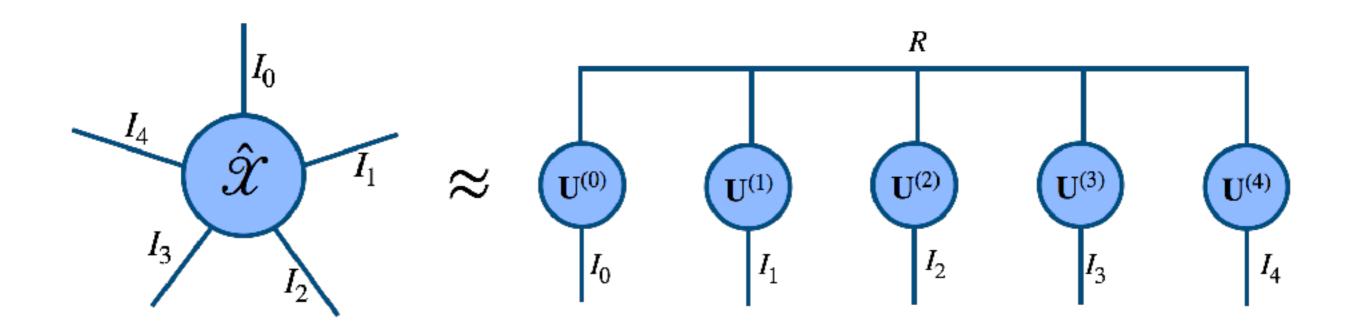
From matrix to tensor

- Matrix decomposition is not unique
- Tensor decomposition unique under mild conditions
 - → Identifiability
- Almost all tensor problems are NP-hard…
- Good algorithms to solve them heuristically

$$\hat{\mathcal{X}} \in \mathbb{R}^{I,J,K}$$

$$\hat{\mathcal{X}} = \sum_{k=0}^{R-1} \mathbf{u}_k^{(0)} \circ \mathbf{u}_k^{(1)} \circ \mathbf{u}_k^{(2)}$$
rank-1 components





$$\hat{\mathcal{X}} \in \mathbb{R}^{I,J,K}$$

$$\hat{\mathcal{X}} = \sum_{k=0}^{R-1} \lambda \mathbf{u}_k^{(0)} \circ \mathbf{u}_k^{(1)} \circ \mathbf{u}_k^{(2)}$$
rank-1 components
rank-R tensor

- Scaling ambiguity: equivalent to choosing units (e.g. for student, scale grade between 1 and 100)
- Permutation between rank-1 components gives same result

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rank-1 components
rank-R tensor

Collect factors in matrices:

$$\mathbf{U}^{(0)} = \begin{bmatrix} \mathbf{u}_0^{(0)}, & \mathbf{u}_1^{(0)}, & , \cdots, \mathbf{u}_{R-1}^{(0)} \end{bmatrix} \in \mathbb{R}^{I,R}$$

$$\mathbf{U}^{(1)} = \begin{bmatrix} \mathbf{u}_0^{(1)}, & \mathbf{u}_1^{(1)}, & , \dots, \mathbf{u}_{R-1}^{(1)} \end{bmatrix} \in \mathbb{R}^{J,R}$$

$$\mathbf{U}^{(2)} = \begin{bmatrix} \mathbf{u}_0^{(2)}, & \mathbf{u}_1^{(2)}, & , \dots, \mathbf{u}_{R-1}^{(2)} \end{bmatrix} \in \mathbb{R}^{K,R}$$

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Problem can be rewritten as:

$$\hat{\mathcal{X}} = [|\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{U}^{(2)}|]$$

Khatri-Rao product

Khatri-Rao = column-wise Kronecker product
 => defined for matrices with same number of columns

$$A \in \mathbb{R}^{m,R}, B \in \mathbb{R}^{n,R}$$

$$\mathbf{A} \odot \mathbf{B} = \begin{bmatrix} \mathbf{A}_{:,0} \otimes \mathbf{B}_{:,0}, & \mathbf{A}_{:,1} \otimes \mathbf{B}_{:,1}, & \cdots, & \mathbf{A}_{:,R} \otimes \mathbf{B}_{:,R}, \end{bmatrix} \in \mathbb{R}^{mn,R}$$

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$$(1) \quad (\mathbf{A} \odot \mathbf{B})^{\top} (\mathbf{A} \odot \mathbf{B}) = \mathbf{A}^{\top} \mathbf{A} * \mathbf{B}^{\top} \mathbf{B}$$

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(2)
$$(\mathbf{A} \odot \mathbf{B})^{\dagger} = ((\mathbf{A}^{\mathsf{T}} \mathbf{A}) * (\mathbf{B}^{\mathsf{T}} \mathbf{B}))^{-1} (\mathbf{A} \odot \mathbf{B})^{\mathsf{T}}$$

$$\hat{\mathcal{X}} \in \mathbb{R}^{I,J,K}$$

$$\hat{\mathcal{X}} = [|\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{U}^{(2)}|]$$

Collect factors in matrices:

$$\mathbf{U}^{(0)} = \begin{bmatrix} \mathbf{u}_0^{(0)}, & \mathbf{u}_1^{(0)}, & , \cdots, \mathbf{u}_{R-1}^{(0)} \end{bmatrix} \in \mathbb{R}^{I,R}$$

$$\mathbf{U}^{(1)} = \begin{bmatrix} \mathbf{u}_0^{(1)}, & \mathbf{u}_1^{(1)}, & , \dots, \mathbf{u}_{R-1}^{(1)} \end{bmatrix} \in \mathbb{R}^{J,R}$$

$$\mathbf{U}^{(2)} = \begin{bmatrix} \mathbf{u}_0^{(2)}, & \mathbf{u}_1^{(2)}, & , \dots, \mathbf{u}_{R-1}^{(2)} \end{bmatrix} \in \mathbb{R}^{K,R}$$

Unfoldings can be expressed as khatri-rao product of the factors:

$$\hat{\mathcal{X}}_{[0]} = \mathbf{U}^{(0)} \begin{pmatrix} \mathbf{U}^{(1)} & \odot & \mathbf{U}^{(2)} \end{pmatrix}^{\mathsf{T}}$$

$$\hat{\mathcal{X}}_{[1]} = \mathbf{U}^{(1)} \begin{pmatrix} \mathbf{U}^{(0)} & \odot & \mathbf{U}^{(2)} \end{pmatrix}^{\mathsf{T}}$$

$$\hat{\mathcal{X}}_{[2]} = \mathbf{U}^{(2)} \begin{pmatrix} \mathbf{U}^{(0)} & \mathbf{o} & \mathbf{U}^{(1)} \end{pmatrix}^\mathsf{T}$$

$$\begin{split} & \min_{\hat{\mathcal{X}}'} \|\hat{\mathcal{X}} - \hat{\mathcal{X}}'\|_F \\ &= & \min_{\hat{\mathcal{X}}'} \|\hat{\mathcal{X}} - [\|\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{U}^{(2)}\|] \|_F \end{split}$$

Frobenius norm:

$$\|\mathcal{X}\|_{F} = \sqrt{\sum_{i_{0}=0}^{I_{0}} \sum_{i_{1}=1}^{I_{1}} \cdots \sum_{i_{N}=0}^{I_{N}} x_{i_{0}i_{1}\cdots i_{N}}^{2}}$$

$$\begin{split} & \min_{\hat{\mathcal{X}}'} \|\hat{\mathcal{X}} - \hat{\mathcal{X}}'\|_F \\ &= & \min_{\hat{\mathcal{X}}'} \|\hat{\mathcal{X}} - [|\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{U}^{(2)}|] \|_F \end{split}$$

- Alternating Least-Square: update one factors at a time, fix all others
- Rewrite the problem in term of the unfolding
- problem becomes linear least squares

Refresher on Linear Least Squares

$$-\mathbf{X}^{\mathsf{T}}\mathbf{Y} + \mathbf{X}^{\mathsf{T}}\mathbf{X}\boldsymbol{\beta} = 0 \qquad \boldsymbol{\beta} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{Y}$$

Refresher on Linear Least Squares

$$\mathbf{Y} \in \mathbb{R}^{N,O}, \mathbf{X} \in \mathbb{R}^{N,F}, \beta \in \mathbb{R}^{F,O}$$

$$\min_{\mathbf{X}} \|\mathbf{Y}^{\top} - \boldsymbol{\beta}^{\top} \mathbf{X}^{\top} \|_{F}$$

$$\beta = \mathbf{Y}^{\mathsf{T}} \mathbf{X} \left(\mathbf{X}^{\mathsf{T}} \mathbf{X} \right)^{-1}$$

$$(\mathbf{X}^{\mathsf{T}})^{\dagger}$$

$$\min_{\mathbf{U}^{(0)}} \| \underbrace{\hat{\mathcal{X}}_{[0]}}_{\mathbf{Y}^{\mathsf{T}}} - \underbrace{\mathbf{U}^{(0)}}_{\beta^{\mathsf{T}}} \underbrace{\left(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)}\right)^{\mathsf{T}}}_{\mathbf{X}^{\mathsf{T}}} \|_{F}$$

$$\beta = \mathbf{Y}^{\mathsf{T}} \mathbf{X} \left(\mathbf{X}^{\mathsf{T}} \mathbf{X} \right)^{-1}$$
$$\underbrace{(\mathbf{X}^{\mathsf{T}})^{\dagger}}$$

$$\mathbf{U}^{(0)} = \hat{\mathcal{X}}_{[0]} \left[\left(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)} \right)^{\mathsf{T}} \right]^{\dagger}$$

$$\min_{\mathbf{U}^{(0)}} \| \hat{\mathcal{X}}_{[0]} - \mathbf{U}^{(0)} \left(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)} \right)^{\mathsf{T}} \|_F$$

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$$\mathbf{U}^{(0)} = \hat{\mathcal{X}}_{[0]} \left[\left(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)} \right)^{\mathsf{T}} \right]^{\dagger}$$
 We can do better!

Khatri-Rao product properties

$$A \in \mathbb{R}^{m,R}, B \in \mathbb{R}^{n,R}$$

$$\mathbf{A} \odot \mathbf{B} = \begin{bmatrix} \mathbf{A}_{:,0} \otimes \mathbf{B}_{:,0}, & \mathbf{A}_{:,1} \otimes \mathbf{B}_{:,1}, & \cdots, & \mathbf{A}_{:,R} \otimes \mathbf{B}_{:,R}, \end{bmatrix} \in \mathbb{R}^{mn,R}$$

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$$\mathbf{U}^{(0)} = \hat{\mathcal{X}}_{[0]} \left(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)} \right) \left[(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)})^{\mathsf{T}} (\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)}) \right]^{-1}$$

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$$\mathbf{U}^{(0)} = \hat{\mathcal{X}}_{[0]} \left(\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)} \right) \left[(\mathbf{U}^{(1)})^{\mathsf{T}} (\mathbf{U}^{(1)}) * (\mathbf{U}^{(2)})^{\mathsf{T}} (\mathbf{U}^{(2)}) \right]^{-1}$$

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- Rank of a tensor: smallest number of rank 1 tensors that generate the tensor as their sum
- No algorithm to determine rank (NP-hard)
- For third order tensor of size I x J x K:
 rank <= min(IJ, IK, JK)

- Kruskal rank: maximum r such that every subset of r columns of A is linearly independent.
- For 3rd order decomposition, with factor matrices, A, B and C, sufficient condition for unicity of rank-R CP:

$$krank(A) + krank(B) + krank(C) \ge 2R + 2$$

 Mild condition if rank not too high: true in general (non-degenerate case)

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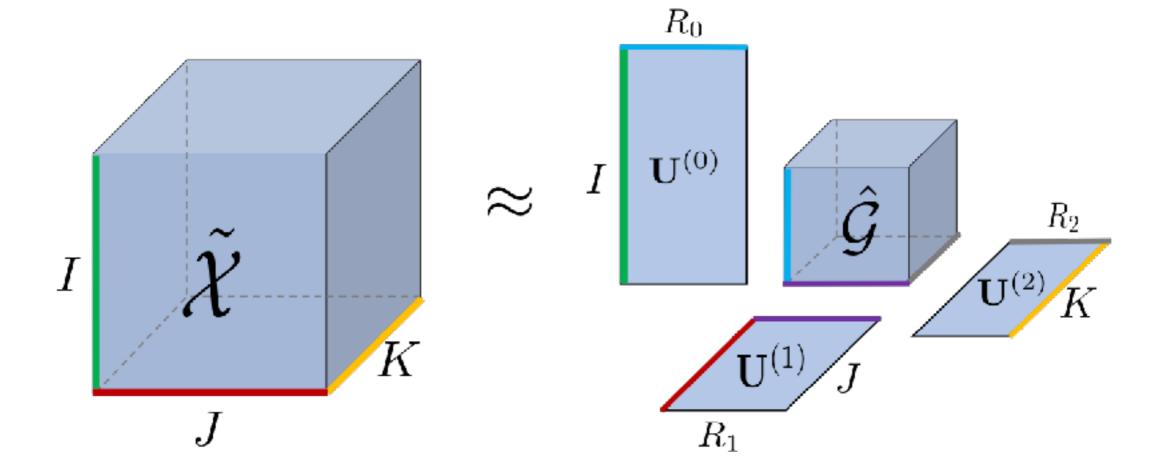
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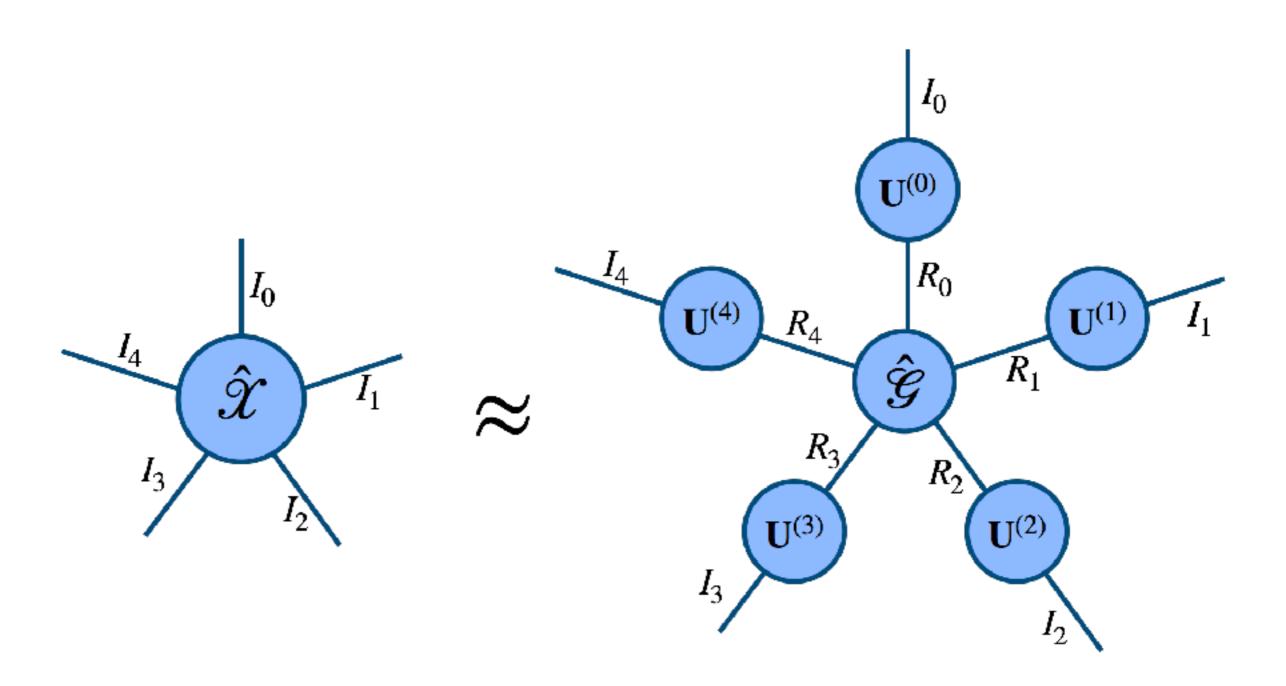
- Mild condition if rank not too high: true in general (non-degenerate case)
- Sufficient condition in general:

$$\sum_{k=0}^{N} \operatorname{krank}(\mathbf{U}^{(k)}) \ge 2R + N$$

$$\hat{\mathcal{X}} \in \mathbb{R}^{I,J,K}$$

$$\hat{\mathcal{X}} = \hat{\mathcal{G}} \times_0 \mathbf{U}^{(0)} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)}$$





$$\hat{\mathcal{X}} = \hat{\mathcal{G}} \times_0 \mathbf{U}^{(0)} \times_1 \mathbf{U}^{(1)} \times \cdots \times_N \mathbf{U}^{(N)}$$

$$\hat{\mathcal{X}} \in \mathbb{R}^{I_0,I_1,\cdots,I_N}$$

$$\hat{\mathcal{G}} \in \mathbb{R}^{R_0,R_1,\cdots,R_N}$$

$$\mathbf{U}^{(0)} \in \mathbb{R}^{I_0, R_0}, \mathbf{U}^{(1)} \in \mathbb{R}^{I_1, R_1}, \dots, \mathbf{U}^{(N)} \in \mathbb{R}^{I_N, R_N},$$

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• Short form: $\hat{\mathcal{G}} \times_0 \mathbf{U}^{(0)} \times_1 \mathbf{U}^{(1)} \times \cdots \times_N \mathbf{U}^{(N)} = [|\hat{\mathcal{G}}; \mathbf{U}^{(0)}, \cdots, \mathbf{U}^{(N)}|]$

Tucker decomposition

$$\hat{\mathcal{X}} = \hat{\mathcal{G}} \times_0 \mathbf{U}^{(0)} \times_1 \mathbf{U}^{(1)} \times \cdots \times_N \mathbf{U}^{(N)}$$

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- Equivalent: $\hat{\mathcal{X}} = \hat{\mathcal{G}} \left(\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \cdots, \mathbf{U}^{(N)} \right)$

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- We can isolate the core and the factors by considering vectorized expression and unfoldings:

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- We can isolate the core and the factors by considering vectorized expression and unfoldings:

$$vec(\hat{\mathcal{X}}) = \left(\mathbf{U}^{(0)} \otimes \cdots \otimes \mathbf{U}^{(N)}\right) vec(\hat{\mathcal{G}})$$

$$\hat{\mathcal{X}}_{[n]} = \mathbf{U}^{(n)} \hat{\mathcal{G}}_{[n]} \left(\mathbf{U}^{(0)} \otimes \cdots \mathbf{U}^{(n-1)} \otimes \mathbf{U}^{(n+1)} \otimes \cdots \otimes \mathbf{U}^{(N)} \right)^{\mathsf{T}}$$

Higher Order SVD

$$\hat{\mathcal{X}} = \hat{\mathcal{G}} \times_0 \mathbf{U}^{(0)} \times_1 \mathbf{U}^{(1)} \times \cdots \times_N \mathbf{U}^{(N)}$$

• For n=0, ...N:

$$\mathbf{U}^{(n)} = R_n$$
 leading left singular vectors of $\hat{\mathcal{X}}_{[n]}$
Truncated SVD

End for

•
$$\hat{\mathcal{G}} = \hat{\mathcal{X}} \times_0 \mathbf{U}^{(0)^T} \times_1 \mathbf{U}^{(1)^T} \times \cdots \times_N \mathbf{U}^{(N)^T}$$

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Tucker via ALS (Higher-Order Orthogonal Iteration)

Use SVD to compute orthonormal factors

$$\hat{\mathcal{X}} = \hat{\mathcal{G}} \times_0 \mathbf{U}^{(0)} \times_1 \mathbf{U}^{(1)} \times \cdots \times_N \mathbf{U}^{(N)}$$

- While not converged:
 - For n=0, ...N:

$$\hat{\mathcal{Y}} = \hat{\mathcal{X}} \times_0 \mathbf{U}^{(0)^T} \times_1 \mathbf{U}^{(1)^T} \times \cdots \times_{n-1} \mathbf{U}^{(n-1)^T} \times_{n+1} \mathbf{U}^{(n+1)^T} \times \cdots \times_N \mathbf{U}^{(N)^T}$$

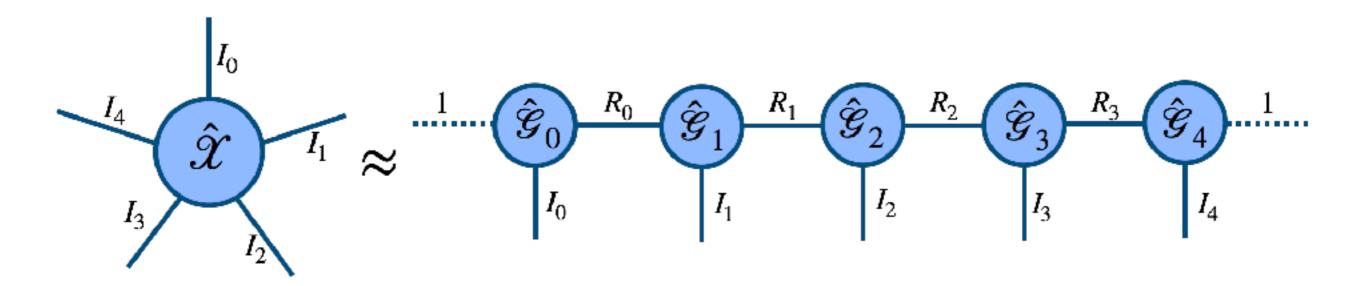
$$\mathbf{U}^{(n)} = R_n \text{ leading left singular vectors of } \hat{\mathcal{Y}}_{[n]}$$

End for

$$\hat{\mathcal{G}} = \hat{\mathcal{X}} \times_0 \mathbf{U}^{(0)^T} \times_1 \mathbf{U}^{(1)^T} \times \cdots \times_N \mathbf{U}^{(N)^T}$$

MPS / T-Train

- Physics: Matrix Product State
- Machine Learning: Tensor-Train (I. V. Oseledets)



MPS / T-Train

$$\hat{\mathcal{X}} \in \mathbb{R}^{I_0,I_1,\cdots,I_N}$$
, Ranks R_0,\cdots,R_N , $R_0=R_N=1$

$$\hat{\mathscr{C}} = \hat{\mathscr{X}}$$

$$\mathbf{C} = \mathbf{reshape}(\hat{\mathscr{C}}, R_{k-1} \times I_k, -1)$$

C = USV, keep first R_k components of U

$$\hat{\mathcal{G}}_k = \mathbf{reshape}(\mathbf{U}[:,:k], [R_{k-1}, I_k, R_k])$$

$$\mathbf{C} = \mathbf{S}\mathbf{V}^{\mathsf{T}}$$

$$\mathbf{C} = \mathbf{S}\mathbf{V}^{\mathsf{T}}$$

$$\hat{\mathscr{G}}_N = \mathbf{C}$$

Tensor decompositions

- Many others (Hierachical Tucker, DEDICOM, PARAFAC2, ...)
- Excellent surveys:
 - Tamara G. Kolda and Brett W. Bader. Tensor decompositions and applications. SIAM REVIEW, 51(3):455–500, 2009.
 - Sidiropoulos, N.D., De Lathauwer, L., Fu, X., Huang, K., Papalexakis, E.E. and Faloutsos, C., 2017. Tensor decomposition for signal processing and machine learning. IEEE Transactions on Signal Processing, 65(13), pp.3551-3582.

Tensor decompositions

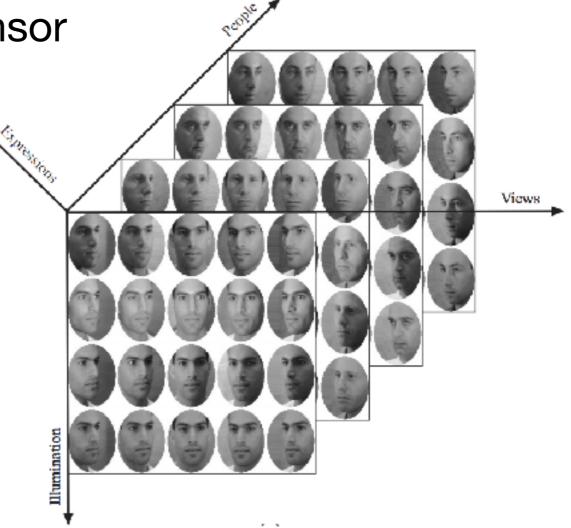
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- Some notable examples:

TensorFaces

 Arrange image of faces in a tensor (e.g. subject x illumination x expression x pixels)

Can be used for recognition

 Can remove effect (e.g. illumination from faces)



M. Alex O. Vasilescu and Demetri Terzopoulos, Multilinear Analysis of Image Ensembles: TensorFaces, ECCV'02

M. Alex O. Vasilescu and Demetri Terzopoulos, Multilinear Subspace Analysis of Image Ensembles, CVPR'03

Method of Moments

- Pearson: find parameters (of models) consistent with observed moments: $\mathbb{E}[X], \mathbb{E}[X^2], \mathbb{E}[X^3], \cdots$
- Topic modelling: moments represent probabilities of occurrence of words, co-occurence, etc..
- By decomposing the moment tensors, we can recover the parameters (here, the rank of the tensor corresponds to the number of topics)

A Anandkumar, R Ge, D Hsu, SM Kakade, M Telgarsky, Tensor Decompositions for Learning Latent Variable Models, JMLR, 2014

Expressiveness of deep nets

- Equivalence between networks and tensor factorisation
- Shallow networks <-> CP decomposition
- Deeper networks correspond to hierarchical Tucker

Nadav Cohen, Or Sharir, Amnon Shashua,

On the Expressive Power of Deep Learning: A Tensor Analysis, 2016



Any questions?

