Tutorial on MATLAB for tensors and the Tucker decomposition

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Workshop on Tensor Decomposition and Applications
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Outline

- Part I
  - Basics of N-way arrays
    - Creating a tensor in MATLAB
    - Tensor multiplication
    - Matricizing a tensor
  - Tensor decompositions
    - What is the SVD of a tensor?
    - PARAFAC model
    - Tucker model
- Part II
  - Computing tensor decompositions
    - Rank-1 approximation
    - Tucker via HO-SVD
    - Tucker via ALS
  - The core array in the Tucker decomposition
  - Working with sparse tensors in MATLAB

MATLAB Tensor Classes

- Enables working with tensors in their native format
  - As tensors rather than as matrices or vectors
- Previewed at last year's workshop in Palo Alto
  - Lots of helpful suggestions from the participants
- Since submitted for publication
  - More helpful suggestions from the referees
- See also the N-way toolbox by Andersson and Bro (2000)

- We provide 4 MATLAB classes
  - **`tensor`**
  - **`tensor_as_matrix`**
  - **`cp_tensor`**
  - **`tucker_tensor`**
- Functions that are part of these classes will be highlighted in red

Download newest MATLAB tensor class and paper at:
http://csmr.ca.sandia.gov/~tgkolda/pubs/index.html#SAND2004-5187

Unzip and add directory to MATLAB path via addpath command.

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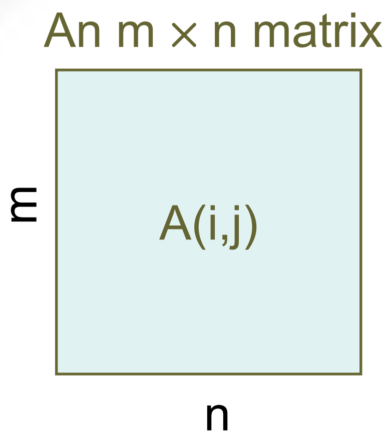
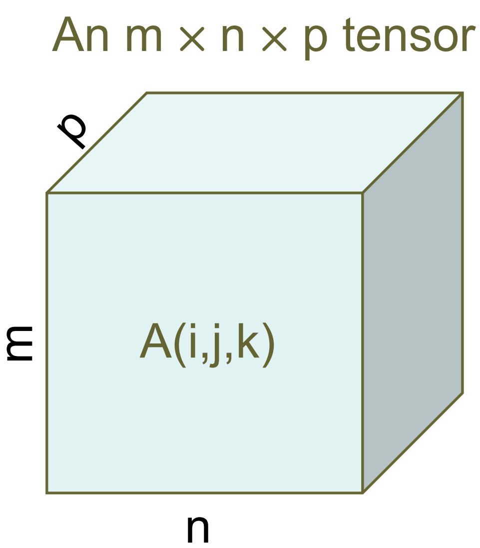
The Basics

A tensor is a multidimensional array





- Other names for tensors…
  - Multi-way array
  - N-way array
- Applications of SVD-like tensor decompositions
  - Image Compression
  - Data Mining
  - Psychometrics
  - Chemometrics
- The order of a tensor is the number of dimensions (a.k.a. ways or modes)
  - Scalar = tensor of order 0
  - Vector = tensor of order 1
  - Matrix = tensor of order 2

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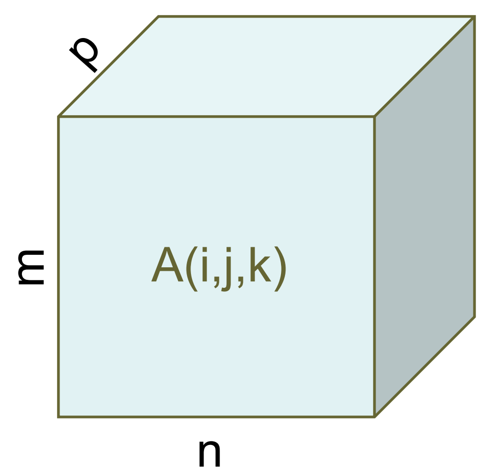
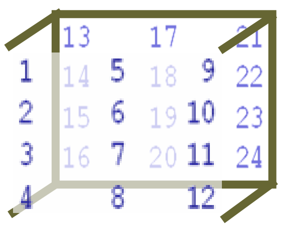
Creating a tensor in MATLAB

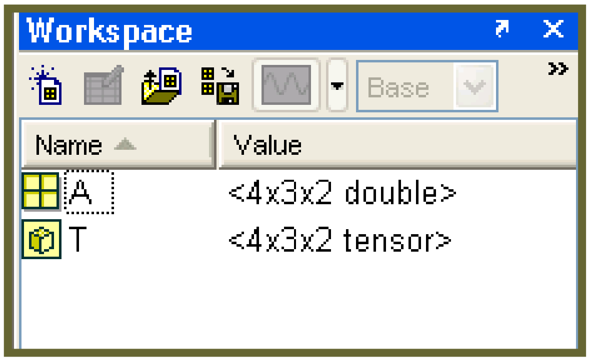
An m × n × p tensor



- MATLAB natively stores tensors as multidimensional arrays (MDAs)
  - `>> A = reshape(1:24, [4 3 2]);`
- The **tensor** class extends the MDA capabilities
  - `>> T = tensor(A) % convert`
  - ```
    T is a tensor of size 4 x 3 x 2
    T.data =
    (:,:,1) =
         1     5     9
         2     6    10
         3     7    11
         4     8    12
    (:,:,2) =
        13    17    21
        14    18    22
        15    19    23
        16    20    24
    ```
  - `>> T + T`
  - `>> T .* T`



Symbol is apropos!



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    ```

Aside: Trailing singleton dimensions

- An MDA does not explicitly track *trailing* singleton dimensions
  - Only non-singleton trailing dimensions are used in the calculation of **`ndims`**
  - Extra trailing singleton dimensions are added as needed, e.g., for **`size`**
- The **`tensor`** object, on the other hand, explicitly tracks its size, including trailing singleton dimensions
  - Constructor needs explicit size if there are trailing dimensions

```
>> A = rand(4,3,2,1);
>> ndims(A)
3
>> size(A,5)
1
>> T = tensor(A);
>> ndims(T)
3
T = tensor(A,[4,3,2,1]);
>> ndims(T)
4
>> size(T,5)
error
```

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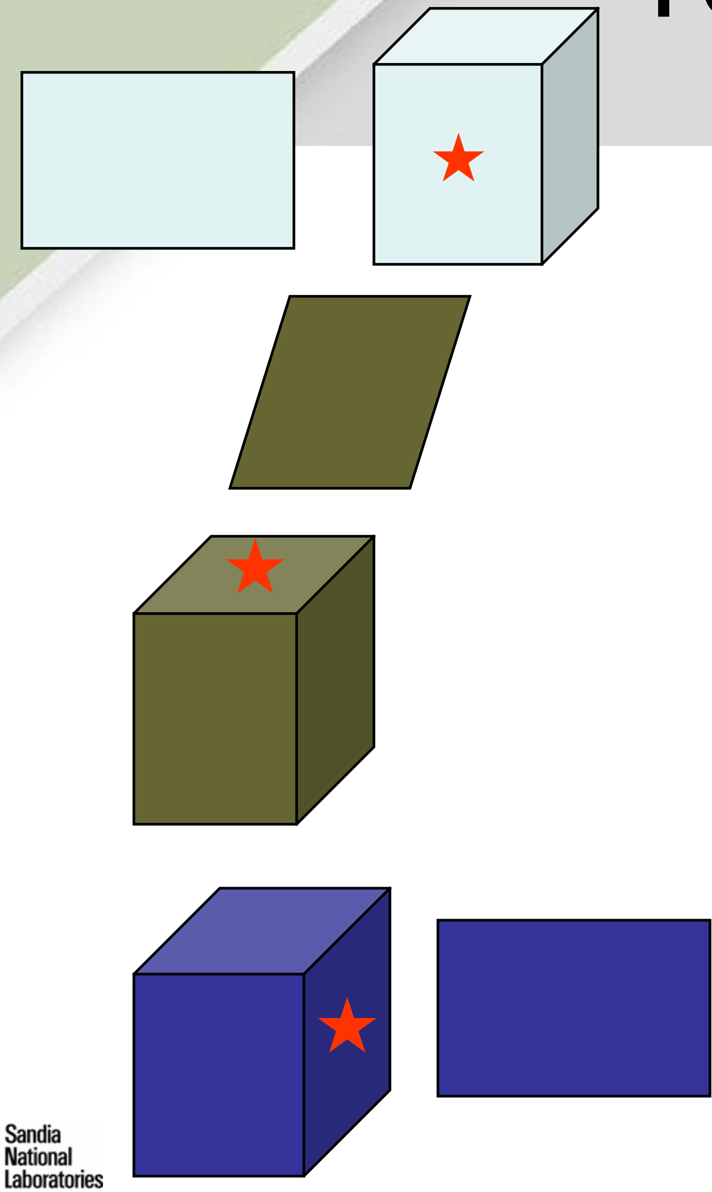
Tensor Multiplication



- Two important special cases
  - Tensor-Matrix
  - Tensor-Vector
- General
  - Tensor-Tensor

From Kruskal (1977) for 3rd order tensors:

Now we introduce multiplication of an array by a matrix, whose product in general is an array. Since an array has three indices, it can be multiplied from three sides: we shall write

$$UX, \qquad \overset{V}{X}, \qquad XW$$

to indicate the three kinds of products: these indicate

$$\sum_i u_{i'i} x_{ijk}, \qquad \sum_j v_{j'j} x_{ijk}, \qquad \sum_k w_{k'k} x_{ijk}.$$

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Tensor-Matrix Multiplication

- Let A be an m x n x p tensor
- Let U be a q x m matrix
- Let V be a r x n matrix
- Mode-n multiplication means to multiply the matrix times the tensor in the n^th mode

$$B = A \times_1 U$$

$$(B)_{\ell jk} = \sum_{i=1}^{m} A_{ijk} U_{\ell i}$$

Alternate Notation: $B = A \bullet_1 U$

- `>> A = tensor(rand(4,3,2));`
- `>> U = rand(3,4);`

$$B = A \times_1 U$$

- `>> B = ttm(A,U,1);`
- `>> size(B)`
- `3 3 2` (size q x n x p)
- `>> V = rand(2,3);`

$$B = A \times_1 U \times_2 V$$

- `>> B = ttm(A,{U,V},[1,2]);`
- `>> size(B)`
- `3 2 2` (size q x r x p)

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Tensor-Vector Multiplication

- Let A be an m x n x p tensor
- Let u be an m-vector
- Let v be an n-vector

$$B = A \bar{\times}_1 u$$

$$(B)_{jk} = \sum_{i=1}^{m} A_{ijk} u_i$$

<u>Note</u>: The same symbol is often used for both tensor-matrix and tensor-vector.

- `>> A = tensor(rand(4,3,2));`
- `>> u = rand(4,1);`

$$B = A \bar{\times}_1 u$$

- `>> B = ttv(A,u,1);`
- `>> size(B)`
- `3 2` (size n x p)
- `>> v = rand(3,1);`

$$B = A \bar{\times}_1 u \bar{\times}_2 v$$

- `>> B = ttv(A,{u,v},[1,2]);`
- `>> size(B)`
- `2` (size p)

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Sequence Multiplication Notation

- We often want to compute a tensor A times a sequence of matrices (or vectors) in all modes but one
- E.g., Multiply a 4th order tensor in all modes but the 3rd
  - $A \times_1 U_1 \times_2 U_2 \times_4 U_4$
  - $A \times_{-3} \{U\}$
- We can do the same with vectors as well
  - $A \bar{\times}_1 u_1 \bar{\times}_2 u_2 \bar{\times}_4 u_4$
  - $A \bar{\times}_{-3} \{u\}$
- Notation is also useful in algorithm descriptions

- Create a tensor and some matrices
  - `>> A = tensor(rand(4,3,2,2));`
  - `>> for i = 1:4, U{i} = rand(2,size(A,i)); end;`
- The following produce equivalent results
  - `>> ttm(A, {U{1}, U{2}, U{4}},[1 2 4])`
  - `>> ttm(A,U,[1 2 4])`
  - `>> ttm(A, U, -3)`

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Tensor-Tensor Multiplication

- Let A be an 4 x 2 x 3 tensor of all ones
  - `>> A = tensor(ones(4,2,3))`
- Let B be an 3 x 4 x 2 tensor
  - `>> B = tensor(rand(3,4,2))`
- Inner Product
  - `>> R = ttt(A,A,1:3)`
  - `24` (scalar)
- Outer product
  - `>> R = ttt(A,B);`
  - `>> size(R)`
  - `4 2 3 3 4 2`
- General multiplication along a subset of dimensions
  - `>> R = ttt(A,B,[1,3], [2,1]);`
  - `>> size(R)`
  - `2 2`

Aside: `ttt` is the kernel for `ttm` and `ttv`.

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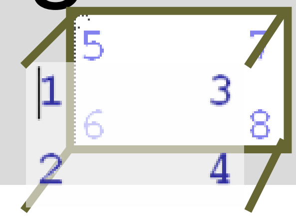
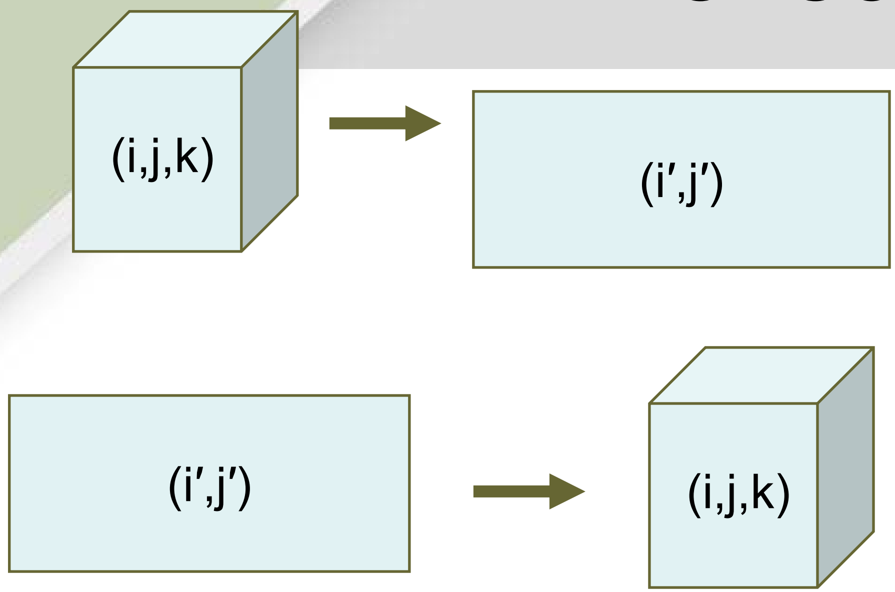
Matricize: Converting a Tensor to a Matrix



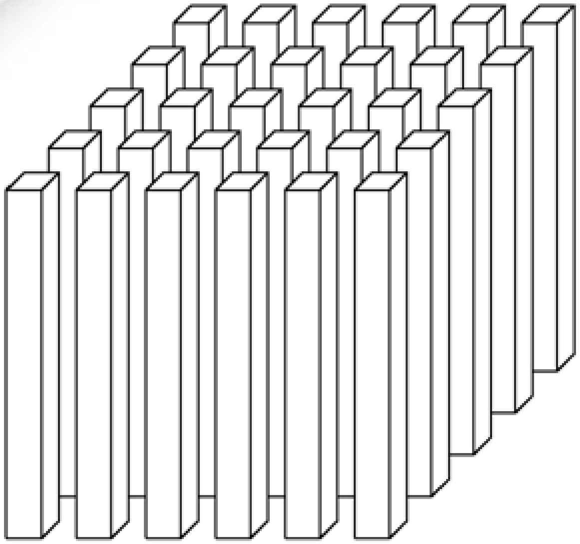


- Important Special Case
  - $A_{(n)}$ = matrix form of a tensor where the n^{th} dimension maps to the rows of the matrix
  - Also called “unfolding”
- Reverse matricize is also possible, provided that we know the mapping

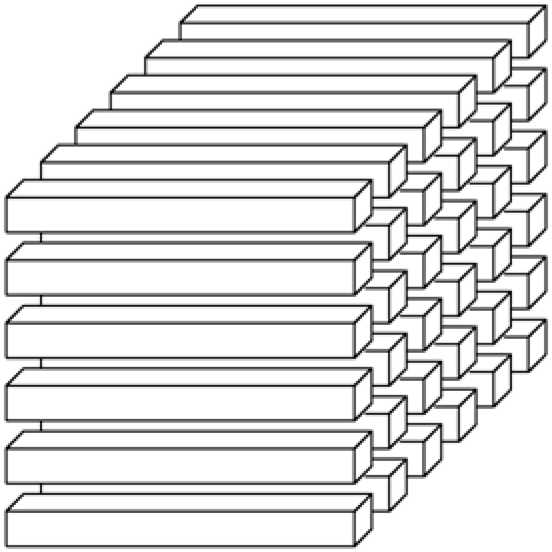
```
>> A=tensor(reshape(1:8,
   [2 2 2]));
>> tensor_as_matrix(A,1)
     1     3     5     7
     2     4     6     8
>> tensor_as_matrix(A,2)
     1     2     5     6
     3     4     7     8
>> tensor_as_matrix(A,3)
     1     2     3     4
     5     6     7     8
>> tensor_as_matrix(A,[1 2]);
   % Try for fun…
```

Tensor “Fibers”

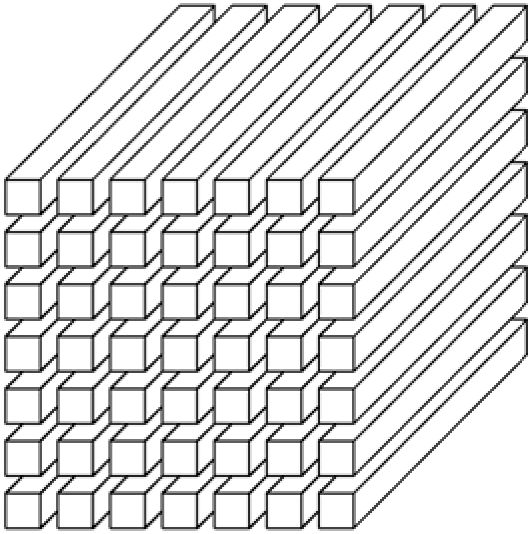
Another view of matricization is lining up the tensor fibers from a particular dimension.



Column fibers comprise columns of $A_{(1)}$



Row fibers comprise columns of $A_{(2)}$



Tube fibers comprise columns of $A_{(3)}$

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Why Matricize?

$$B = A \times_n U$$

$$B_{(n)} = U A_{(n)}$$

- Few software products support n-way arrays
- E.g., MATLAB added MDAs only recently
- Representation as a matrix may be the only option
  - In fact, our `ttt` operator converts the tensors to matrices to do the multiplication
- *However, rearranging the elements for different matricizations can be expensive and may be unnecessary*

Two Useful Facts for n-Mode Multiplication

- Identity 1: $A \times_n (UV) = A \times_n V \times_n U$
- Identity 2: Let U be a p x q matrix with full column rank. If $B = A \times_n U$ then $A = B \times_n Z$ where Z is the q x p left inverse of U
- Example: If U has orthonormal columns, then $B = A \times_n U \Rightarrow A = B \times_n U^T$
- Proofs follow immediately from $B = A \times_n U \Leftrightarrow B_{(n)} = U A_{(n)}$

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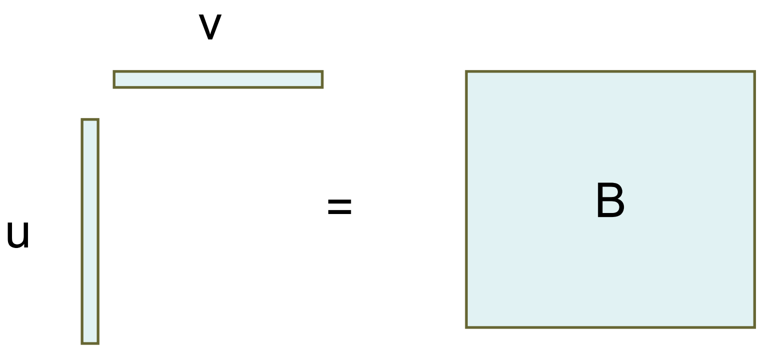
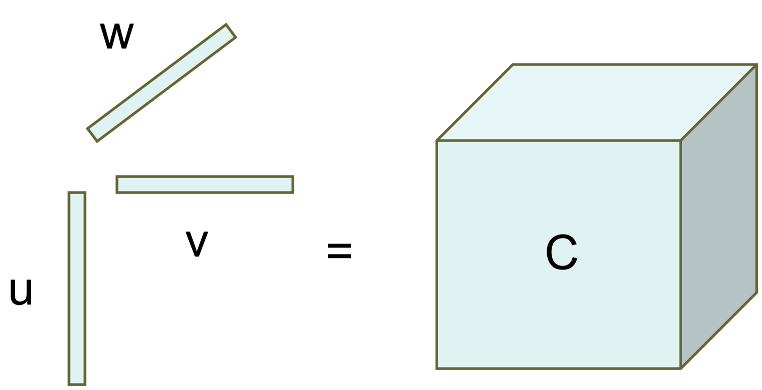
Tensor Decompositions

Building Blocks: Rank-1 Tensors

- 2D
  - $B = u \circ v = u\, v^T$
  - $B(i,j) = u(i) \cdot v(j)$
- 3D (a.k.a. triad)
  - $C = u \circ v \circ w$
  - $C(i,j,k) = u(i) \cdot v(j) \cdot w(k)$
- 4D (a.k.a. 4-ad or N-ad)
  - $D = u \circ v \circ w \circ x$
  - $D(i,j,k,l) = u(i) \cdot v(j) \cdot w(k) \cdot x(l)$
- Alternate notation:
  - $u \otimes v$ or $u \Delta v$





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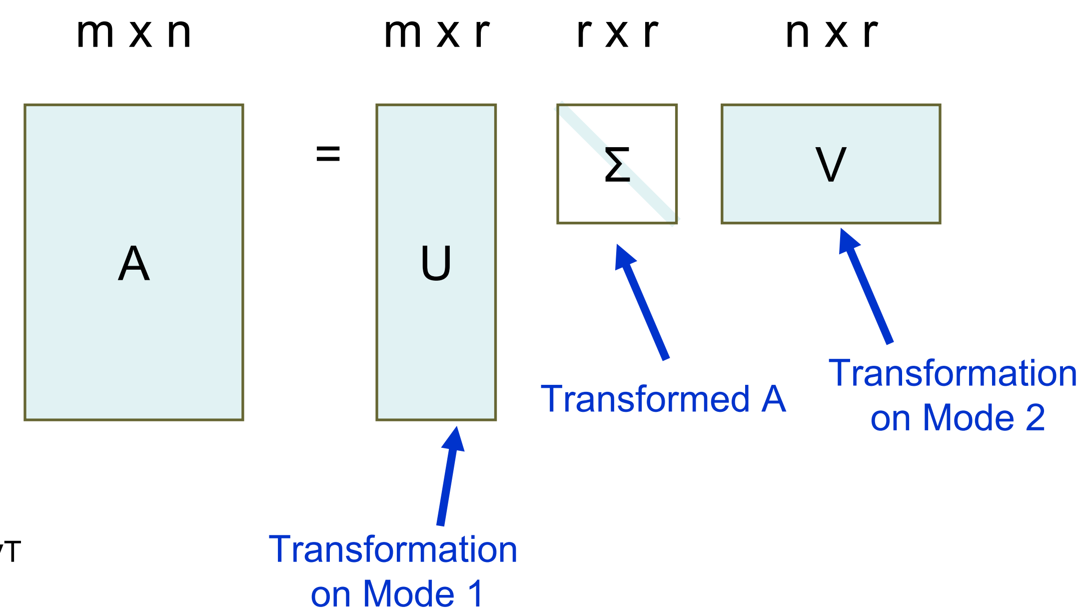
Matrix SVD:
$A = \Sigma \times_1 U \times_2 V$

i^{th} column of U

$$A = \sum_{i=1}^{r} \sigma_{ii}\, u_i \circ v_i$$

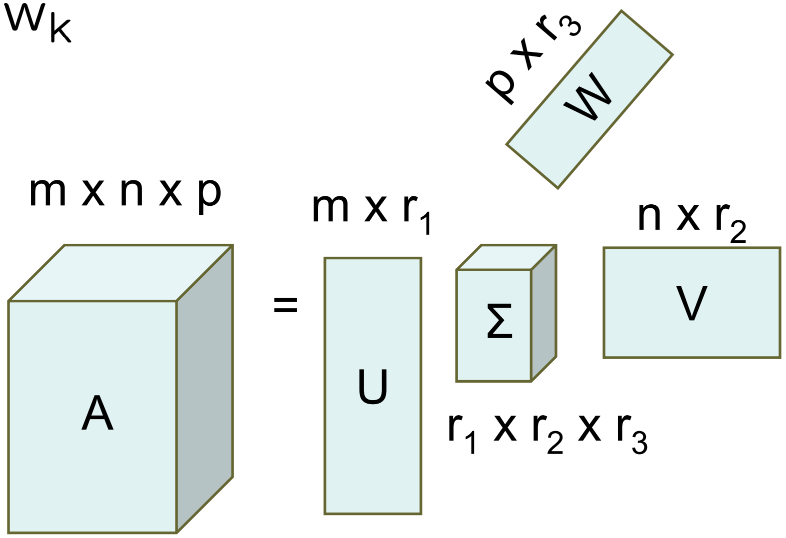
i^{th} column of V



- SVD or PCA: $A = U \Sigma V^T$
- Σ is a diagonal matrix
- Columns of U, V are orthonormal
- Two-way PCA: does not always require Σ to be diagonal (e.g., Henrion '94)
- ICA: U and V need not be be orthonormal

Tensor SVD: $A = \Sigma \times_1 U \times_2 V \times_3 W$

$$A = \sum_{i=1}^{r_1} \sum_{j=1}^{r_2} \sum_{k=1}^{r_3} \sigma_{ijk}\, u_i \circ v_j \circ w_k$$



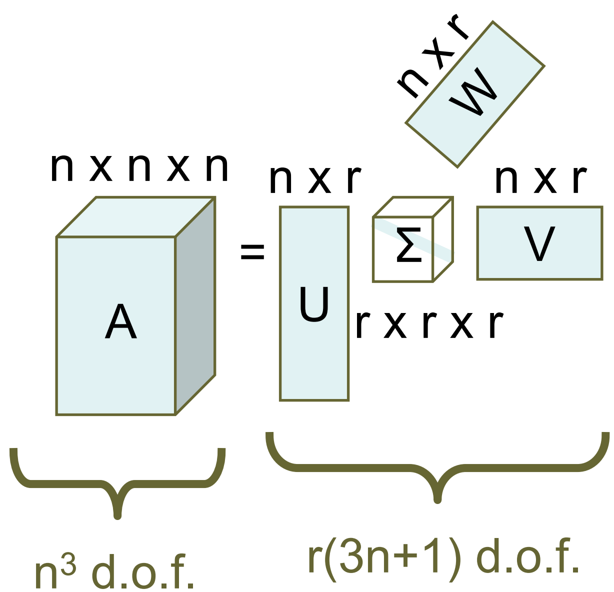
- Σ is the core tensor
- U, V, W are the components or factors
- In general, can have either
  - Diagonal core **or**
  - Orthonormal columns in components

Why can't we have both?

- Let A be a tensor of size n x n x n
- Suppose we do have both
  - diagonal Σ
  - orthogonal U,V,W
- Diagonal Σ yields

$$A = \sum_{i=1}^{r} \sigma_{iii}\, u_i \circ v_i \circ w_i$$

- Orthogonal U,V,W gives $r \leq n$
- $\Rightarrow$ Right-hand-side has only has $O(n^2)$ d.o.f.

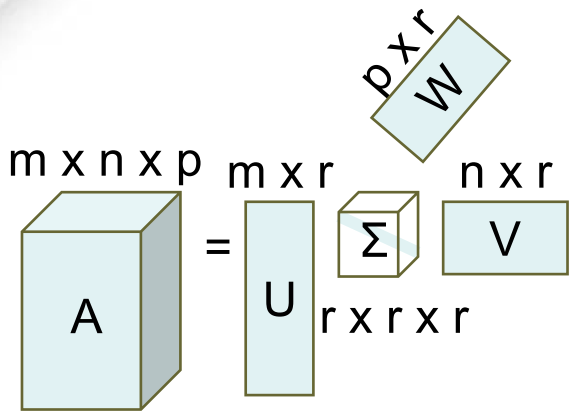


Two Choices

1. Diagonal Σ **or**
2. Orthogonal U,V,W

Diagonal Σ

CANDECOMP-PARAFAC (CP) Decomposition



$$A = \Sigma \times_1 U \times_2 V \times_3 W$$

$$A = \sum_{i=1}^{r} \sigma_{iii}\, u_i \circ v_i \circ w_i$$

- CANDECOMP = Canonical Decomposition of Carroll and Chang (1970)
- PARAFAC = Parallel Factors of Harshman (1970)
- a.k.a. Tensor Canonical Decomposition
- Columns of U, V, and W are not orthogonal
- If r is *minimal*, then r is called the rank of the tensor (Kruskal 1977)
- Can have rank(A) > min{m,n,p}
- Often guaranteed to be a unique rank decomposition!
- Abbreviation CP follows Kiers (2000)

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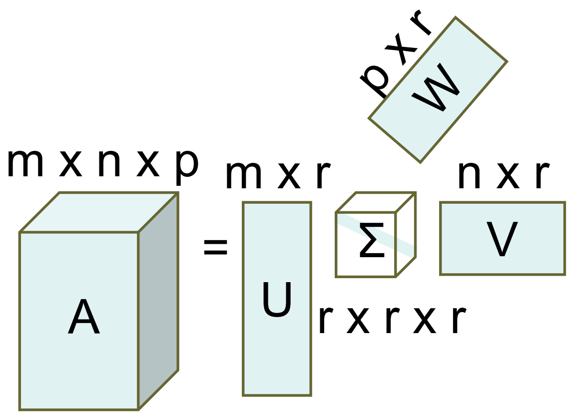
CP Tensors in MATLAB

$$A = \Sigma \times_1 U \times_2 V \times_3 W$$

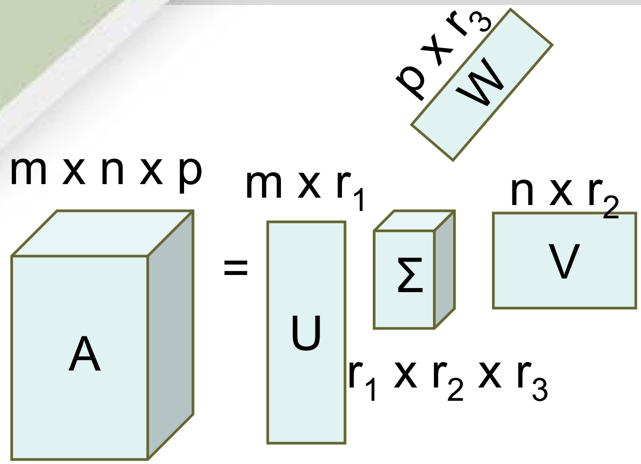
$$A = \sum_{i=1}^{r} \sigma_{iii}\, u_i \circ v_i \circ w_i$$




```
>> r = 2;
>> U = rand(2,r);
>> V = rand(3,r);
>> W = rand(2,r);
>> A = cp_tensor({U,V,W})
A is a CP tensor of size 2 x 3 x 2
A.lambda =
    1
    1
A.U{1} =
    0.5485    0.5973
    0.2618    0.0493
A.U{2} =
    0.5711    0.7400
    0.7009    0.4319
    0.9623    0.6343
A.U{3} =
    0.0839    0.9159
    0.9455    0.6020
```

U,V,W Orthogonornal

Tucker Decomposition



$$A = \Sigma \times_1 U \times_2 V \times_3 W$$

$$A = \sum_{i=1}^{r_1} \sum_{j=1}^{r_2} \sum_{k=1}^{r_3} \sigma_{ijk}\, u_i \circ v_j \circ w_k$$

- Proposed by Tucker (1966)
- a.k.a. three-mode factor analysis, three-mode PCA, orthogonal array decomposition
- Sum of all possible combination of vectors from U,V,W
- Σ is <u>not</u> diagonal
- Not unique

Σ is not free:

$$\Sigma = A \times_1 U^T \times_2 V^T \times_3 W^T$$

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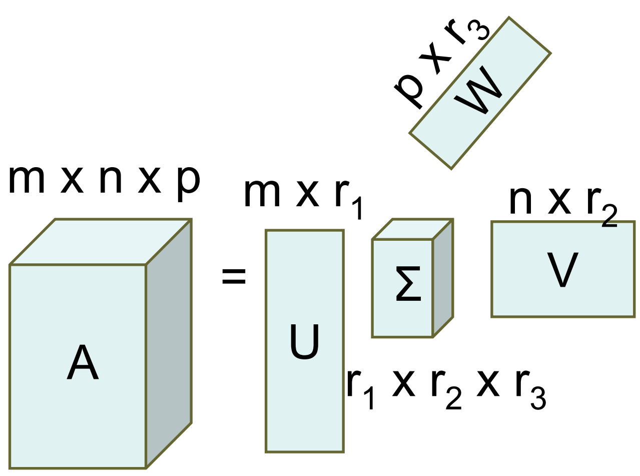
Tucker Tensors in MATLAB

$$A = \Sigma \times_1 U \times_2 V \times_3 W$$

$$A = \sum_{i=1}^{r_1} \sum_{j=1}^{r_2} \sum_{k=1}^{r_3} \sigma_{ijk}\, u_i \circ v_j \circ w_k$$




```
>> siz = [2 3 2];
>> core = tensor(rand(2,2,1),[2 2 1]);
>> % Pick orthogonal matrices
>> for i = 1:3, [U{i},junk] =
    qr(rand(siz(i), size(core,i)),0);
    end
>> A = tucker_tensor(core,U)
A is a Tucker tensor of size 2 x 3 x 2
A.lambda is a tensor of size 2 x 2 x 1
A.lambda.data =
    0.2009    0.6262
    0.2731    0.5369
A.U{1} =
    0.0595    0.2713
    0.0890    0.4091
A.U{2} =
    0.4740    0.3290
    0.9090    0.4782
    0.5962    0.5972
A.U{3} =
    0.1614
    0.8295
```

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MATLAB Notes for Tucker and CP

- Access the core array (a vector for CP and a tensor for Tucker)
  - `>> A.lambda`
  - ```
    ans is a tensor of size 2 x 2 x 1
    ans.data =
        0.2009    0.6262
        0.2731    0.5369
    ```
- Access the n^th matrix
  - `>> A.U{2}`
  - ```
    ans =
        0.4740    0.3290
        0.9090    0.4782
        0.5962    0.5972
    ```
- Convert to a tensor object
  - `>> full(A)`
  - ```
    ans is a tensor of size 2 x 3 x 2
    ans.data =
    (:,:,1) =
        0.0163    0.0267    0.0259
        0.0245    0.0403    0.0390
    (:,:,2) =
        0.0837    0.1374   0.1332
        0.1261    0.2069    0.2005
    ```

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    ```

End of Part I

Questions?

Computing Tensor Decompositions

Focus is on Tucker – PARAFAC is left to Richard Harshman's tutorial later today.

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Rank-1 Approximation

- Goal: Find vectors u,v,w that minimize

$$\|A - \lambda \, \mathsf{u} \circ \mathsf{v} \circ \mathsf{w}\|_F^2 = \sum_{ijk} \left(\mathsf{A}_{ijk} - \lambda \, \mathsf{u}_i \mathsf{v}_j \mathsf{w}_k \right)^2$$

- WLOG, assume ‖ u ‖ = ‖ v ‖ = ‖ w ‖ = 1, and

$$\lambda = \mathsf{A} \,\bar{\times}_1\, \mathsf{u} \,\bar{\times}_2\, \mathsf{v} \,\bar{\times}_3\, \mathsf{w}$$

- Can repeatedly compute the best rank-1 approximation to the residual to get a “greedy PARAFAC” model

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Best Rank-1 Approximation

Optimal answer for fixed v & w

For k = 1, 2, . . .

$$\tilde{u}^{(k+1)} = A \bar{\times}_2 v^{(k)} \bar{\times}_3 w^{(k)}$$
$$\tilde{v}^{(k+1)} = A \bar{\times}_1 \tilde{u}^{(k+1)} \bar{\times}_3 w^{(k)}$$
$$\tilde{w}^{(k+1)} = A \bar{\times}_1 \tilde{u}^{(k+1)} \bar{\times}_2 \tilde{v}^{(k+1)}$$

$$u^{(k+1)} = \tilde{u}^{(k+1)} / \|\tilde{u}^{(k+1)}\|$$
$$v^{(k+1)} = \tilde{v}^{(k+1)} / \|\tilde{v}^{(k+1)}\|$$
$$w^{(k+1)} = \tilde{w}^{(k+1)} / \|\tilde{w}^{(k+1)}\|$$

$$\lambda^{(k+1)} = A \bar{\times}_1 u^{(k+1)} \bar{\times}_2 v^{(k+1)} \bar{\times}_3 w^{(k+1)}$$

end

Given Tensor A.
Find best rank-1 approximation:
$\lambda\, u \circ v \circ w$

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Higher Order Power Method: De Lathauwer, De Moor, Vandewalle (2000)

Power Method in MATLAB

```
% A = 3-way tensor
for i = 1:maxits
  u = ttv(A,{v,w},-1);
  v = ttv(A,{u,w},-2);
  w = ttv(A,{u,v},-3);
  u = u / norm(u);
  v = v / norm(v);
  w = w / norm(w);
  s = ttv(A,{u,v,w});
end
B = cp_tensor(s,{u,v,w})
C = tucker_tensor(tensor(s,[1 1 1]),{u,v,w});
```

See **examples/hopm.m** for full method.

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HO-SVD (Tucker1)

Given Tensor A.
Find a rank-(r_1,r_2,r_3) Tucker Decomposition

$\Sigma \times_1 U \times_2 V \times_3 W$

U has r_1 columns
V has r_2 columns
W has r_3 columns

$$
\begin{aligned}
U &= r_1 \text{ left singular vectors of } A_{(1)} \\
V &= r_2 \text{ left singular vectors of } A_{(2)} \\
W &= r_3 \text{ left singular vectors of } A_{(3)} \\
\Sigma &= A \times_1 U^T \times_2 V^T \times_3 W^T
\end{aligned}
$$

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Tucker (1966), De Lathauwer, De Moor, Vandewalle (2000)

MATLAB HO-SVD

```
% A = tensor
% r1,r2,r3 = desired ranks
[U,xx,zz] = svds(double(tensor_as_matrix(A,1)),r1)
[V,xx,zz] = svds(double(tensor_as_matrix(A,2)),r2)
[W,xx,zz] = svds(double(tensor_as_matrix(A,3)),r3)
S = ttm(A,{U',V',W'})
B = tucker_tensor(S,{U,V,W});
```

Best Rank-(r_1,r_2,r_3) Approximation

Given Tensor A.
Find best approximation:

$\Sigma \times_1 U \times_2 V \times_3 W$

U, V, W orthogonal
U has r_1 columns
V has r_2 columns
W has r_3 columns

Optimal answer for fixed V & W

For $k = 1, 2, \ldots$

$$X^{(k+1)} = A \times_2 V^{(k)^T} \times_3 W^{(k)^T}$$
$$U^{(k+1)} = \text{first } r_1 \text{ left singular vectors of } X_{(1)}^{(k+1)}$$

$$Y^{(k+1)} = A \times_1 U^{(k+1)^T} \times_3 W^{(k)^T}$$
$$V^{(k+1)} = \text{first } r_2 \text{ left singular vectors of } Y_{(2)}^{(k+1)}$$

$$Z^{(k+1)} = A \times_1 U^{(k+1)^T} \times_2 V^{(k+1)^T}$$
$$W^{(k+1)} = \text{first } r_3 \text{ left singular vectors of } Z_{(3)}^{(k+1)}$$

$$\Sigma^{(k+1)} = A \times_1 U^{(k+1)^T} \times_2 V^{(k+1)^T} \times_3 W^{(k+1)^T}$$

end

TUCKALS3 or HOOI: Kroonenberg and de Leeuw (1980), Kapteyn et al. (1986), De Lathauwer et al. (2000)

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```
% A = tensor
% r1,r2,r3 = desired ranks
for i = 1:maxits
  T = ttm(A,{V',W'},-1);
  [U,xx,zz] = svds(double(tensor_as_matrix(T,1)),r1);
  T = ttm(A,{U',W'},-2);
  [V,xx,zz] = svds(double(tensor_as_matrix(T,2)),r2);
  T = ttm(A,{U',V'},-3);
  [W,xx,zz] = svds(double(tensor_as_matrix(T,3)),r3);
end
S = ttm(A,{U',V',W'})
B = tucker_tensor(S,{U,V,W});
```

See `examples/hooi.m` for full method.

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Optimizing the Core

- Tucker decomposition is not uniquely determined
- Can freely multiply the components U,V,W by non-singular matrices R,S,T
  - This in turn changes the core Σ

$$\boxed{A = \Sigma \times_1 U \times_2 V \times_3 W}$$

Equivalent

$$\boxed{\begin{aligned} A &= \tilde{\Sigma} \times_1 (RU) \times_2 (SV) \times_3 (TW) \\ \tilde{\Sigma} &= \Sigma \times_1 R^{-1} \times_2 S^{-1} \times_3 T^{-1} \end{aligned}}$$

- Freedom can be used to modify Σ so that it has meaning
  - Maximize diagonal
  - Maximize variance (i.e., tends toward either 0 or 1 entries)
- See, e.g.,
  - Kiers (1992, 1997, 1998), Henrion (1993)

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Sparse Tensors in MATLAB

(time permitting)

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Storing Sparse N-Way Data

- Sparse Matrix Storage Schemes
  - For m x n matrix with q nonzeros
  - Compressed sparse row (CSR)
    - For each entry, store its column index and value
    - Store the start of each row plus the end of the last row
    - Storage = 2q + m + 1
    - Easy to pull out a row, hard to pull out a column
    - Can do analogous Compress Sparse Column (CSC)
    - Generally considered the most efficient storage format
  - Coordinate format
    - Store row and column index along with each value
    - Storage = 3q

- Sparse Multiway Data Storage Schemes
  - For m x n x p with q nonzeros
  - Compressed sparse mode
    - For each entry, stores its mode-n index and value
    - Store and end (per mode)
    - Storage = 2q + m(n+1) + 1
    - Various efficiencies are possible (e.g., skipping)
  - Store $A_{(3)}$ in CSR format
    - Storage = 2q + mn + 1
  - Store $A_{(3)}$ in CSC format
    - Storage = 2q + p + 1
  - Coordinate format
    - Store all mode indices with each value
    - Storage = 4q

Our choice

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Computing with Coordinate Format: $A \times_2 u$

- Let A be a 3rd order tensor of size m x n x p with q nonzeros
  - `Aidx` = indices stored as a q x 3 array
  - `Aval` = values stored as a q x 1 array
- Let u be an n-vector
  - `u` = n x 1 array
- How do we calculate $B = A \times_2 u$?
  - Without explicit for-loops!

```
[subs,junk,loc] =
   unique(Aidx(:,[1,3]),
   'rows');
vals = accumarray(loc,
   Avals .* u(Aidx(:,2)));
nz = find(vals);
Bsubs = subs(nz,:);
Bvals = vals(nz);
```

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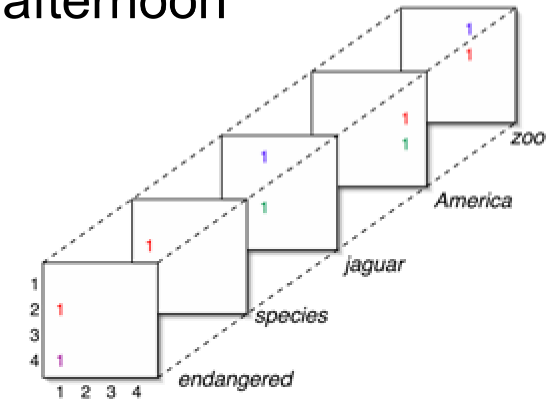
Computational Efficiency

- In MATLAB, need to avoid explicitly looping over data
- Make extensive use of built-in MATLAB functions such as…
  - ismember
  - setdiff
  - unique
  - accumarray
  - cumprod / cumsum
  - sort / sortrows

Is anyone interested in a MATLAB toolbox for sparse tensors?

- Have been able to run a greedy PARAFAC and similar algorithms on problems of size
  - 50k x 50k x 70k
  - ½ million nonzeros
- See Brett's talk on Friday afternoon



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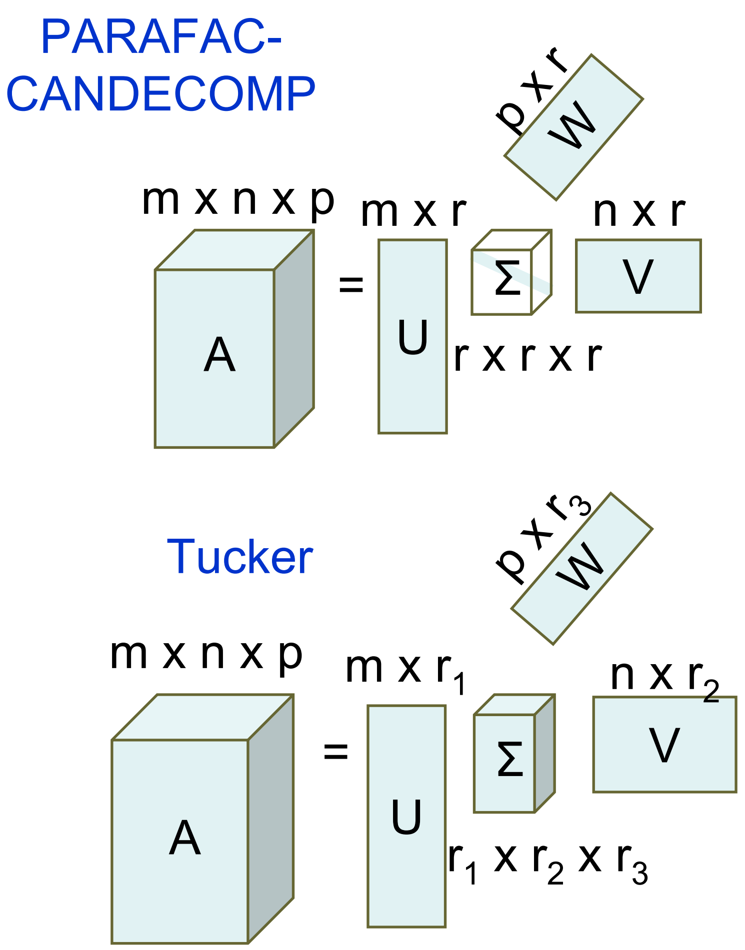
Summary & References

Summary

- Part I
  - Basics of N-way arrays
  - Tensor decompositions
- Part II
  - Computing tensor decompositions
  - Choosing the core in the Tucker decomposition
  - Sparse tensors



Thanks for your attention.
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