# Tensor Computations and Applications in Data Mining 

Lars Eldén

Department of Mathematics
Linköping University, Sweden
Joint work with Berkant Savas
SIAM AM July 2008

## Are Tensors too Difficult?

Murray \& Rice, Differential geometry and statistics, 1993:

$$
\begin{equation*}
\left.\xi(\chi)_{j_{1} \ldots j_{s}}^{i_{1} \ldots i_{r}}=\xi(\theta)\right)_{l_{1} \ldots l_{s}, \ldots k_{s}}^{k_{r}} \frac{\partial \chi^{i_{1}}}{\partial \theta^{k_{1}}} \cdots \frac{\partial \chi^{i_{r}}}{\partial \theta^{k_{r}}} \frac{\partial \theta^{l_{1}}}{\partial \chi^{k_{1}}} \cdots \frac{\partial \theta^{j_{1}}}{\partial \chi^{j_{s}}} \tag{8.7.1}
\end{equation*}
$$

Classically it would have been said that the tensor transforms by this rule. It is horrible formulae like this that have given tensor analysis a bad name.
"... the manipulation of matrices is a hundred times better supported in our brains and in our software tools than that of tensors."
( N . Trefethen, Maxims about numerical mathematics, science, computers, and life on earth)

## Notation and Concepts

We need a notational and conceptual framework that

- exhibits the structure of the problems
- is independent of the order of the tensor, or easily generalizable
- allows the formulation and implementation of algorithms

Q: Can we find such a framework in math books on tensor calculus?

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A: NO! (in general), because we are asking different questions now. Many fundamental mathematical problems are open!

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Tensor methods have been used since the 1960's in psychometrics and chemometrics! Only recently in numerical community.
Applications in signal processing and various areas of data mining.

> Recent survey:
> Tammy Kolda \& Brett Bader, Tensor Decompositions and Applications, SIAM Review, to appear. (Download from Tammy's web page)

## Outline

(1) Introduction

- Tensor data
- Singular Value Decomposition
- Digits
(2) Tensor concepts
- Matrix-tensor multiplication
- Inner Product and Norm
- Contractions
(3) HOSVD
(4) Best Approximation
- Grassmann Optimization
- Gradient
- Hessian
- Numerical Examples
(5) Sparse Tensors: Krylov Methods

6 Conclusions

## Multi-Mode Data:

Example: Classification of hand-written digits
pixel mode, 400 pixels
3 -tensor $\mathcal{D}$ with digit mode, $\sim 1000$ digits per class class mode, 10 classes


All digits of one class represented by a slice

## Two Aspects of SVD: Expansion - Decomposition

1. Expansion in terms of rank-1 matrices:

$$
x=\sum_{i=1}^{n} \sigma_{i} u_{i} v_{i}^{T}=|\square+|=+\cdots
$$

2. Matrix decomposition: $\mathbb{R}^{m \times n} \ni X=U \Sigma V^{\top}$

$$
\begin{aligned}
& \square X=\begin{array}{l}
0 \\
V^{\top} \\
m \times n
\end{array} \\
& m \times m \times n
\end{aligned}
$$

## Tensor Expansion in Rank-1 Terms



- Parafac/Candecomp/Kruskal: Harshman, Caroll, Chang 1970
- Numerous papers in psychometrics and chemometrics
- From a mathematical point of view: difficult problem, sometimes ill-posed, see De Silva and Lim 2006.
- From the point of view of applications: very useful! (Rasmus Bro's talk)


## Tensor Decomposition: Tucker Model



- Tucker 1964, numerous papers in psychometrics and chemometrics
- De Lathauwer, De Moor, Vandewalle, SIMAX 2000: notation, theory.
- The matrices $U^{(i)}$ are usually orthogonal.

This talk: Tucker model for 3-tensors only!

## Classification of Handwritten Digits


"Model problem" in pattern recognition

## HOSVD for Data Reduction

pixel mode, 400 pixels digit mode, $\sim 1000$ digits per class class mode, 10 classes


D
digits
Cf. low-rank approximation of matrix by SVD: $A \approx U_{k} \Sigma_{k} V_{k}^{T}$

## Project all Digits to Low Dimension


$\left(P^{\top}\right)_{1} \cdot \mathcal{D}$
Each column is a digit in low dimension

$\mathcal{F}$


D bases

Slice $\mu$ of $\mathcal{F}$ is a basis for class $\mu$
Compute the SVD of each slice: $\mathcal{F}(:, .,, \mu)=U^{\mu} \Sigma^{\mu}\left(V^{\mu}\right)^{T}$ and use $k$ columns, $U_{k}^{\mu}$, as basis vectors.

## Classification with HOSVD Compression

- Training phase:
( Collect the training digits into a tensor $\mathcal{D}$.
(2) Compute the HOSVD of $\mathcal{D}$.
(3) Compute the low rank "basis" tensor $\mathcal{F}=\left(P^{T}\right)_{1} \cdot \mathcal{D}$.
(4) Compute and store the basis matrices $B^{\mu}=U_{k}^{\mu}$ for each class.
- Test phase: For each test digit $d$
(1) Project $d=P^{T} d$.
(2) Compute the residuals $R(\mu)=\left\|\left(I-B^{\mu}\left(B^{\mu}\right)^{T}\right) d\right\|, \mu=1, \ldots, 10$.
(8) Determine $\mu_{\text {min }}=\operatorname{argmin}_{\mu} R(\mu)$ and classify $d$ as $\mu_{\text {min }}$.


## Classification results: US Postal Service Database



Figure: Error rates for different compressions (> 97.8\%), and basis dimension.

## Mode-/ Multiplication of a Tensor by a Matrix

Assume that dimensions are such that all operations are well-defined. Mostly 3-tensors. Lim's notation. (No standard notation yet)

$$
\mathcal{B}=(X)_{1} \cdot \mathcal{A}, \quad \mathcal{B}(i, j, k)=\sum_{\nu=1}^{n} x_{i \nu} a_{\nu j k}
$$

All column vectors are multiplied by the matrix $X$.
Multiplication in all modes at the same time:

$$
\mathcal{B}=(X, Y, Z) \cdot \mathcal{A}, \quad \mathcal{B}(i, j, k)=\sum_{\nu, \mu, \lambda} x_{i \nu} y_{j \mu} z_{k \lambda} a_{\nu \mu \lambda}
$$

For convenience we write

$$
\mathcal{B}=\left(X^{T}, Y^{T}, Z^{T}\right) \cdot \mathcal{A}=\mathcal{A} \cdot(X, Y, Z)
$$

## Inner Product and Norm

Inner product (contraction: $\mathbb{R}^{n \times n \times n} \rightarrow \mathbb{R}$ )

$$
\langle\mathcal{A}, \mathcal{B}\rangle=\sum_{i, j, k} a_{i j k} b_{i j k}
$$

The Frobenius norm:

$$
\|\mathcal{A}\|=\langle\mathcal{A}, \mathcal{A}\rangle^{1 / 2}
$$

Matrix case

$$
\langle A, B\rangle=\operatorname{tr}\left(A^{T} B\right)
$$

## Partial Contractions

$$
\begin{array}{rlrl}
\mathcal{C} & =\langle\mathcal{A}, \mathcal{B}\rangle_{1}, & c_{j k l m} & =\sum_{\lambda} a_{\lambda j k} b_{\lambda / m}, \\
D & =\langle\mathcal{A}, \mathcal{B}\rangle_{1: 2}, & d_{j k} & =\sum_{\lambda, \mu} a_{\lambda \mu j} b_{\lambda \mu k}, \\
e & =\langle\mathcal{A}, \mathcal{B}\rangle=\langle\mathcal{A}, \mathcal{B}\rangle_{1: 3}, & e & \text { (2-tensor) }, \\
a_{\lambda \mu \nu} b_{\lambda \mu \nu}, & \quad \text { (scalar) }
\end{array}
$$

Notation (3-tensor):

$$
\langle\mathcal{A}, \mathcal{B}\rangle_{1: 2}=\langle\mathcal{A}, \mathcal{B}\rangle_{-3}
$$

## Tensor SVD (HOSVD): $\mathcal{A}=\left(U^{(1)}, U^{(2)}, U^{(3)}\right) \cdot \mathcal{S}$


(1) Compute the SVD of all mode-i vectors
(2) $U^{(i)}$ is left singular matrix of mode $i$
(3) $\mathcal{S}:=\mathcal{A} \cdot\left(U^{(1)}, U^{(2)}, U^{(3)}\right)$

The "mass" of $\mathcal{S}$ is concentrated around the $(1,1,1)$ corner. Not optimal: does not give the solution of $\min _{\operatorname{rank}(\mathcal{B})=\left(r_{1}, r_{2}, r_{3}\right)\|\mathcal{A}-\mathcal{B}\|}$

De Lathauwer et al (2000)

## Best Rank- $\left(r_{1}, r_{2}, r_{3}\right)$ Approximation



Best rank-( $\left.r_{1}, r_{2}, r_{3}\right)$ approximation:

$$
\min _{X, Y, Z, \mathcal{S}}\|\mathcal{A}-(X, Y, Z) \cdot \mathcal{S}\|, \quad X^{\top} X=I, \quad Y^{\top} Y=I, \quad Z^{\top} Z=I
$$

The problem is over-parameterized!

## Best Approximation

$$
\min _{\operatorname{rank}(\mathcal{B})=\left(r_{1}, r_{2}, r_{3}\right)}\|\mathcal{A}-\mathcal{B}\|
$$

is equivalent to

$$
\begin{aligned}
\max _{X, Y, Z} \Phi(X, Y, Z) & =\frac{1}{2}\|\mathcal{A} \cdot(X, Y, Z)\|^{2} \\
& =\frac{1}{2} \sum_{j, k, l}\left(\sum_{\lambda, \mu, \nu} a_{\lambda \mu \nu} x_{\lambda j} y_{\mu k} z_{\nu l}\right)^{2}
\end{aligned}
$$

subject to

$$
X^{\top} X=I_{r_{1}}, \quad Y^{\top} Y=I_{r_{2}}, \quad Z^{\top} Z=I_{r_{3}}
$$

## Grassmann Optimization

The Frobenius norm is invariant under orthogonal transformations:

$$
\Phi(X, Y, Z)=\Phi(X U, Y V, Z W)=\frac{1}{2}\|\mathcal{A} \cdot(X U, Y V, Z W)\|^{2}
$$

for orthogonal $U \in \mathbb{R}^{r_{1} \times r_{1}}, V \in \mathbb{R}^{r_{2} \times r_{2}}$, and $W \in \mathbb{R}^{r_{3} \times r_{3}}$.
Maximize $\Phi$ over equivalence classes

$$
[X]=\{X U \mid U \text { orthogonal }\} .
$$

Product of manifolds: $\operatorname{Gr}^{3}=\operatorname{Gr}\left(J, r_{1}\right) \times \operatorname{Gr}\left(K, r_{2}\right) \times \operatorname{Gr}\left(L, r_{3}\right)$

$$
\max _{(X, Y, Z) \in \mathrm{Gr}^{3}} \Phi(X, Y, Z)=\max _{(X, Y, Z) \in \mathrm{Gr}^{3}} \frac{1}{2}\langle\mathcal{A} \cdot(X, Y, Z), \mathcal{A} \cdot(X, Y, Z)\rangle
$$

## Newton's Method on one Grassmann Manifold

Taylor expansion + linear algebra on tangent space ${ }^{1}$ at $X$

$$
G(X(t)) \approx G(X(0))+\langle\Delta, \nabla G\rangle+\frac{1}{2}\langle\Delta, H(\Delta)\rangle,
$$

Grassmann gradient:

$$
\nabla G=\Pi_{x} G_{X}, \quad\left(G_{x}\right)_{j k}=\frac{\partial G}{\partial x_{j k}}, \quad \Pi_{X}=I-X X^{\top}
$$

The Newton equation for determining $\Delta$ :

$$
\Pi_{X}\left\langle\mathcal{G}_{x x}, \Delta\right\rangle_{1: 2}-\Delta\left\langle X, G_{x}\right\rangle_{1}=-\nabla G, \quad\left(\mathcal{G}_{x x}\right)_{j k l m}=\frac{\partial^{2} G}{\partial X_{j k} \partial X_{l m}}
$$

${ }^{1}$ Tangent space at $X$ : all matrices $Z$ satisfying $Z^{T} X=0$.

## Newton-Grassmann Algorithm on $\mathrm{Gr}^{3}$

Here: local coordinates
Given tensor $\mathcal{A}$ and starting points $\left(X_{0}, Y_{0}, Z_{0}\right) \in \mathrm{Gr}^{3}$
repeat
(1) compute the Grassmann gradient $\nabla \widehat{\Phi}$
(2) compute the Grassmann Hessian $\widehat{\mathcal{H}}$
(3) matricize $\widehat{\mathcal{H}}$ and vectorize $\nabla \widehat{\Phi}$
(4) solve $D=\left(D_{x}, D_{y}, D_{z}\right)$ from the Newton equation
(5) take a geodesic step along the direction $D$, giving new iterates ( $\mathrm{X}, \mathrm{Y}, \mathrm{Z}$ )
until $\|\nabla \widehat{\Phi}\| / \Phi<$ TOL
Implementation using TensorToolbox (Bader/Kolda) and home-made object-oriented Grassmann classes in Matlab

## Newton's method on $\mathrm{Gr}^{3}$

Differentiate $\Phi(X, Y, Z)$ along a geodesic curve $(X(t), Y(t), Z(t))$ in the direction $\left(\Delta_{X}, \Delta_{y}, \Delta_{z}\right)$ :

$$
\frac{\partial x_{s t}}{\partial t}=\left(\Delta_{x}\right)_{s t}
$$

and

$$
\left(\frac{d X(t)}{d t}, \frac{d Y(t)}{d t}, \frac{d Z(t)}{d t}\right)=\left(\Delta_{x}, \Delta_{y}, \Delta_{z}\right)
$$

Since $\mathcal{A} \cdot(X, Y, Z)$ is linear in $X, Y, Z$ separately:

$$
\frac{d(\mathcal{A} \cdot(X, Y, Z))}{d t}=\mathcal{A} \cdot\left(\Delta_{x}, Y, Z\right)+\mathcal{A} \cdot\left(X, \Delta_{y}, Z\right)+\mathcal{A} \cdot\left(X, Y, \Delta_{z}\right)
$$

## First Derivative

$$
\begin{aligned}
\frac{d \Phi}{d t} & =\frac{1}{2} \frac{d}{d t}\langle\mathcal{A} \cdot(X, Y, Z), \mathcal{A} \cdot(X, Y, Z)\rangle=\left\langle\mathcal{A} \cdot\left(\Delta_{x}, Y, Z\right), \mathcal{A} \cdot(X, Y, Z)\right\rangle \\
& +\left\langle\mathcal{A} \cdot\left(X, \Delta_{y}, Z\right), \mathcal{A} \cdot(X, Y, Z)\right\rangle+\left\langle\mathcal{A} \cdot\left(X, Y, \Delta_{z}\right), \mathcal{A} \cdot(X, Y, Z)\right\rangle .
\end{aligned}
$$

We want to write $\left\langle\mathcal{A} \cdot\left(\Delta_{X}, Y, Z\right), \mathcal{A} \cdot(X, Y, Z)\right\rangle$ in the form $\left\langle\Delta_{X}, \Phi_{X}\right\rangle$ Define the tensor $\mathcal{F}=\mathcal{A} \cdot(X, Y, Z)$ and write

$$
\left\langle\mathcal{A} \cdot\left(\Delta_{x}, Y, Z\right), \mathcal{F}\right\rangle=:\left\langle\mathcal{K}_{x}\left(\Delta_{x}\right), \mathcal{F}\right\rangle=\left\langle\Delta_{x}, \mathcal{K}_{x}^{*} \mathcal{F}\right\rangle,
$$

For fixed $Y$ and $Z$ we have a linear operator:

$$
\Delta_{X} \longmapsto \mathcal{K}_{X}\left(\Delta_{X}\right)=\mathcal{A} \cdot\left(\Delta_{X}, Y, Z\right)
$$

## Adjoint Operator

Linear operator:

$$
\Delta_{x} \longmapsto \mathcal{K}_{x}\left(\Delta_{x}\right)=\mathcal{A} \cdot\left(\Delta_{x}, Y, Z\right)
$$

with adjoint

$$
\left\langle\mathcal{K}_{x}\left(\Delta_{x}\right), \mathcal{F}\right\rangle=\left\langle\Delta_{x}, \mathcal{K}_{x}^{*} \mathcal{F}\right\rangle=\left\langle\Delta_{x},\langle\mathcal{A} \cdot(I, Y, Z), \mathcal{F}\rangle_{-1}\right\rangle
$$

where the partial contraction is defined

$$
\langle\mathcal{B}, \mathcal{C}\rangle_{-1}\left(i_{1}, i_{2}\right)=\sum_{\mu, \nu} b_{i_{1} \mu \nu} c_{i_{2} \mu \nu}
$$

## Grassmann Gradient

$X$-part: multiply by $\Pi_{X}=I-X X^{T}$

$$
\begin{aligned}
\Pi_{X} \Phi_{X} & =\Pi_{X}\langle\mathcal{A} \cdot(I, Y, Z), \mathcal{F}\rangle_{-1} \\
& =\langle\mathcal{A} \cdot(I, Y, Z), \mathcal{A} \cdot(X, Y, Z)\rangle_{-1}-X X^{T}\langle\mathcal{A} \cdot(I, Y, Z), \mathcal{F}\rangle_{-1} \\
& =\langle\mathcal{A} \cdot(I, Y, Z), \mathcal{A} \cdot(I, Y, Z)\rangle_{-1} X-X\langle\mathcal{F}, \mathcal{F}\rangle_{-1}
\end{aligned}
$$

Complete gradient (recall $\mathcal{F}=\mathcal{A} \cdot(X, Y, Z)$ ):

$$
\nabla \Phi=\left(\Pi_{X} \Phi_{X}, \Pi_{Y} \Phi_{y}, \Pi_{Z} \Phi_{z}\right)
$$

where

$$
\begin{aligned}
& \Pi_{X} \Phi_{X}=\langle\mathcal{A} \cdot(I, Y, Z), \mathcal{A} \cdot(I, Y, Z)\rangle_{-1} X-X\langle\mathcal{F}, \mathcal{F}\rangle_{-1} \\
& \Pi_{Y} \Phi_{y}=\langle\mathcal{A} \cdot(X, I, Z), \mathcal{A} \cdot(X, I, Z)\rangle_{-2} Y-Y\langle\mathcal{F}, \mathcal{F}\rangle_{-2} \\
& \Pi_{Y} \Phi_{Z}=\langle\mathcal{A} \cdot(X, Y, I), \mathcal{A} \cdot(X, Y, I)\rangle_{-3} Z-Z\langle\mathcal{F}, \mathcal{F}\rangle_{-3}
\end{aligned}
$$

## Second Derivative

$$
\begin{aligned}
& \frac{d^{2} \Phi}{d t^{2}}= \\
& =\left\langle\mathcal{A} \cdot\left(\Delta_{X}, Y, Z\right), \mathcal{A} \cdot\left(\Delta_{X}, Y, Z\right)\right\rangle+\left\langle\mathcal{A} \cdot\left(\Delta_{X}, \Delta_{y}, Z\right), \mathcal{A} \cdot(X, Y, Z)\right\rangle \\
& +\left\langle\mathcal{A} \cdot \cdot\left(\Delta_{X}, Y, Z\right), \mathcal{A} \cdot\left(X, \Delta_{Y}, Z\right)\right\rangle+\left\langle\mathcal{A} \cdot\left(\Delta_{X}, Y, \Delta_{Z}\right), \mathcal{A} \cdot(X, Y, Z)\right\rangle \\
& +\left\langle\mathcal{A} \cdot\left(\Delta_{X}, Y, Z\right), \mathcal{A} \cdot\left(X, Y, \Delta_{z}\right\rangle\right\rangle+\cdots,
\end{aligned}
$$

plus 10 analogous terms.

## Grassmann Hessian

$$
\mathcal{H}(\Delta)=\left(\Phi_{x *}(\Delta), \Phi_{y *}(\Delta), \Phi_{z *}(\Delta)\right): \mathbb{T}^{3} \mapsto \mathbb{T}^{3}
$$

where

$$
\begin{array}{ll}
\Phi_{x *}(\Delta)=\mathcal{H}_{x x}\left(\Delta_{x}\right)+\mathcal{H}_{x y}\left(\Delta_{y}\right)+\mathcal{H}_{x z}\left(\Delta_{z}\right), & \Phi_{x *}(\cdot): \mathbb{T}^{3} \rightarrow \mathbb{T}_{X} \\
\Phi_{y *}(\Delta)=\mathcal{H}_{y x}\left(\Delta_{x}\right)+\mathcal{H}_{y y}\left(\Delta_{y}\right)+\mathcal{H}_{y z}\left(\Delta_{z}\right), & \Phi_{y *}(\cdot): \mathbb{T}^{3} \rightarrow \mathbb{T}_{Y} \\
\Phi_{z *}(\Delta)=\mathcal{H}_{z x}\left(\Delta_{x}\right)+\mathcal{H}_{z y}\left(\Delta_{y}\right)+\mathcal{H}_{z z}\left(\Delta_{z}\right), & \Phi_{z *}(\cdot): \mathbb{T}^{3} \rightarrow \mathbb{T}_{z}
\end{array}
$$

## Grassmann Hessian, "Diagonal Part"

$$
\begin{array}{ll}
\mathcal{H}_{x x}\left(\Delta_{x}\right)=\Pi_{x}\left\langle\mathcal{B}_{x}, \mathcal{B}_{x}\right\rangle_{-1} \Delta_{x}-\Delta_{x}\langle\mathcal{F}, \mathcal{F}\rangle_{-1}, & \mathcal{B}_{x}=\mathcal{A} \cdot(I, Y, Z), \\
\mathcal{H}_{y y}\left(\Delta_{y}\right)=\Pi_{Y}\left\langle\mathcal{B}_{y}, \mathcal{B}_{y}\right\rangle_{-2} \Delta_{y}-\Delta_{y}\langle\mathcal{F}, \mathcal{F}\rangle_{-2}, & \mathcal{B}_{y}=\mathcal{A} \cdot(X, I, Z), \\
\mathcal{H}_{z z}\left(\Delta_{z}\right)=\Pi_{z}\left\langle\mathcal{B}_{z}, \mathcal{B}_{z}\right\rangle_{-3} \Delta_{z}-\Delta_{z}\langle\mathcal{F}, \mathcal{F}\rangle_{-3}, & \mathcal{B}_{z}=\mathcal{A} \cdot(X, Y, I) .
\end{array}
$$

## Grassmann Hessian, "Upper Triangular Part",

$$
\begin{aligned}
\mathcal{H}_{x y}\left(\Delta_{y}\right) & =\Pi_{x}\left(\left\langle\left\langle\mathcal{C}_{x y}, \mathcal{F}\right\rangle_{-(1,2)}, \Delta_{y}\right\rangle_{2,4 ; 1,2}\right. \\
& \left.+\left\langle\left\langle\mathcal{B}_{x}, \mathcal{B}_{y}\right\rangle_{-(1,2)}, \Delta_{y}\right\rangle_{4,2 ; 1,2}\right)
\end{aligned}
$$

where $\mathcal{C}_{x y}=\mathcal{A} \cdot(I, I, Z)$, etc.
4-tensor contracted with a matrix giving a matrix:

$$
\left\langle\left\langle\mathcal{C}_{x y}, \mathcal{F}\right\rangle_{-(1,2)}, \Delta_{y}\right\rangle_{2,4 ; 1,2}
$$

## Illustration of Hessian Computation

## Local coordinates.



## Methods for Best Approximation

- Grassmann-based
(1) Newton (LE, B. Savas)
(2) Trust region/Newton (Ishteva, De Lathauwer et al.)
(3) BFGS quasi-Newton (Savas, Lim)
(4) Limited memory BFGS (Savas, Lim)
- Alternating
(1) HOOI (Kroonenberg, De Lathauwer)


## Numerical Example I



A random tensor $\mathcal{A} \in \mathbb{R}^{20 \times 20 \times 20}$ with random entries $\mathrm{N}(0,1)$ approximated with a rank - $(5,5,5)$ tensor.

## Numerical Example II



A random tensor $\mathcal{A} \in \mathbb{R}^{100 \times 100 \times 100}$ with random entries $\mathrm{N}(0,1)$ approximated with a rank $-(5,10,20)$ tensor.

## Sparse Tensors in Information Sciences

In information sciences the tensors are often sparse:

- Term-document-author (Dunlavy et al)
- Graphs, web link analysis (Kolda et al)

For sparse matrices: Krylov methods give low rank approximations:

$$
A V_{k}=U_{k} H_{k}
$$



The matrix is only used as operator: $u=A v$

## Sparse Tensors

Can we generalize Krylov methods to tensors and obtain low rank approximations?


## Golub-Kahan Bidiagonalization for Rectangular Matrix

- $\beta_{1} u_{1}=b, v_{0}=0$
- for $i=1: k$

$$
\begin{aligned}
& \alpha_{i} v_{i}=A^{T} u_{i}-\beta_{i} v_{i-1}, \\
& \beta_{i+1} u_{i+1}=A v_{i}-\alpha_{i} u_{i}
\end{aligned}
$$

- end

The coefficients $\alpha_{i}$ and $\beta_{i}$ are chosen to normalize the vectors.

## Golub-Kahan Bidiagonalization for Rectangular Matrix

- $\beta_{1} u_{1}=b, v_{0}=0$
- for $i=1: k$

$$
\begin{array}{ll}
\alpha_{i} v_{i}=A^{T} u_{i}-\beta_{i} v_{i-1}, & {\left[\alpha_{i} v_{i}=A \cdot\left(u_{i}\right)_{1}-\beta_{i} v_{i-1},\right]} \\
\beta_{i+1} u_{i+1}=A v_{i}-\alpha_{i} u_{i} & {\left[\beta_{i+1} u_{i+1}=A \cdot\left(v_{i}\right)_{2}-\alpha_{i} u_{i}\right]}
\end{array}
$$

- end

The coefficients $\alpha_{i}$ and $\beta_{i}$ are chosen to normalize the vectors.

## Krylov Method for Tensor Approximation

Arnoldi style (i.e., including Gram-Schmidt orthogonalization)

- Let $u_{1}$ and $v_{1}$ be given
- $h_{111} w_{1}=\mathcal{A} \cdot\left(u_{1}, v_{1}\right)_{1,2}$
- for $\nu=2$ : $m$

$$
\begin{aligned}
& h_{u}=\mathcal{A} \cdot\left(U_{\nu-1}, v_{\nu-1}, w_{\nu-1}\right) \\
& h_{\nu, \nu-1, \nu-1} u_{\nu}=\mathcal{A} \cdot\left(v_{\nu-1}, w_{\nu-1}\right)_{2,3}-U_{\nu-1} h_{u} \\
& h_{v}=\mathcal{A} \cdot\left(u_{\nu}, V_{\nu-1}, w_{\nu-1}\right) \\
& h_{\nu, \nu, \nu-1} v_{\nu}=\mathcal{A} \cdot\left(u_{\nu}, w_{\nu-1}\right)_{1,3}-V_{\nu-1} h_{v} \\
& h_{w}=\mathcal{A} \cdot\left(u_{\nu}, v_{\nu}, W_{\nu-1}\right) \\
& h_{\nu \nu \nu} w_{\nu}=\mathcal{A} \cdot\left(u_{\nu}, v_{\nu}\right)_{1,2}-W_{\nu-1} h_{w}
\end{aligned}
$$

- end

Approximate

$$
\mathcal{A} \approx\left(U_{m}, V_{m}, W_{m}\right) \cdot \mathcal{H}, \quad \mathcal{H}=\left(U_{m}^{T}, V_{m}^{T}, W_{m}^{T}\right) \cdot \mathcal{A}
$$

## Krylov Method for Tensor Approximation

Arnoldi style (i.e., including Gram-Schmidt orthogonalization)

- Let $u_{1}$ and $v_{1}$ be given
- $h_{111} w_{1}=\mathcal{A} \cdot\left(u_{1}, v_{1}\right)_{1,2}$
- for $\nu=2$ : $m$

$$
\begin{aligned}
& h_{u}=\mathcal{A} \cdot\left(U_{\nu-1}, v_{\nu-1}, w_{\nu-1}\right) \\
& h_{\nu, \nu-1, \nu-1} u_{\nu}=\mathcal{A} \cdot\left(v_{\nu-1}, w_{\nu-1}\right)_{2,3}-U_{\nu-1} h_{u} \\
& h_{\nu}=\mathcal{A} \cdot\left(u_{\nu}, V_{\nu-1}, w_{\nu-1}\right) \\
& h_{\nu, \nu, \nu-1} v_{\nu}=\mathcal{A} \cdot\left(u_{\nu}, w_{\nu-1}\right)_{1,3}-V_{\nu-1} h_{v} \\
& h_{w}=\mathcal{A} \cdot\left(u_{\nu}, v_{\nu}, W_{\nu-1}\right) \\
& h_{\nu \nu \nu} w_{\nu}=\mathcal{A} \cdot\left(u_{\nu}, v_{\nu}\right)_{1,2}-W_{\nu-1} h_{w}
\end{aligned}
$$

- end

Approximate

$$
\mathcal{A} \approx\left(U_{m}, V_{m}, W_{m}\right) \cdot \mathcal{H}, \quad \mathcal{H}=\left(U_{m}^{T}, V_{m}^{T}, W_{m}^{T}\right) \cdot \mathcal{A}
$$

## Tensor Krylov Methods

- Many variants are possible: see the talk by Berkant Savas in the session MS117 Friday at 4.30
- Suitable for
- sparse tensors
- tensors whose dimensions vary rapidly (new data)


## Conclusions

- Tensor methods/algorithms without index-wrestling
- Indices hidden using matrix-inspired notation and object-oriented software
- Generalization to higher order tensors is straightforward
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- Many fundamental mathematical and algorithmic problems remain
- Numerous new applications in information sciences
- Tensor algorithms and computations can be (easily) managed if we define the right abstractions!


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