Third-Order Tensor Decompositions and Their Application in Quantum Chemistry

Tyler Ueltschi April 17, 2014

April 17, 2014

Table of Contents

Table of Contents

3rd-Order Tensor

Definition: 3rd-Order Tensor

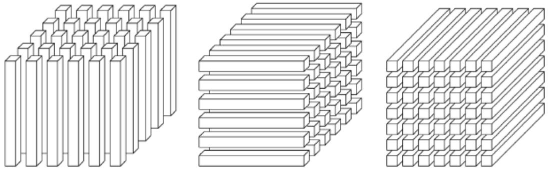
An array of $n \times m$ matrices

3rd-Order Tensor

- 3rd-Order Tensor Definition

Fibers:

458 TAMARA G. KOLDA AND BRETT W. BADER



(a) Mode-1 (column) fibers: $\mathbf{x}_{:jk}$ (b) Mode-2 (row) fibers: $\mathbf{x}_{i:k}$ (c) Mode-3 (tube) fibers: $\mathbf{x}_{ij:}$

Fig. 2.1 *Fibers of a 3rd-order tensor.* [a]

[a] From Bader and Kolda 2009

3rd-Order Tensor

- 3rd-Order Tensor Definition
- Fibers

Slices:

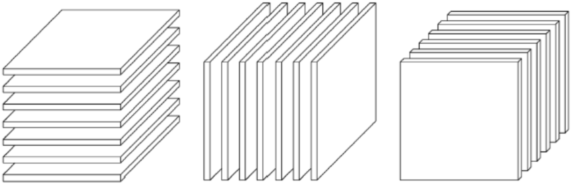


Fig. 2.2 *Slices of a 3rd-order tensor.* [a]

[a] From Bader and Kolda 2009

Table of Contents

Modal Operations

- Modal Operations take Tensors to Matrices

Example: Modal Unfolding

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 13 & 14 & 15 & 16 \\ 17 & 18 & 19 & 20 \\ 21 & 22 & 23 & 24 \end{bmatrix}$$

Modal Operations

- Modal Operations take Tensors to Matrices

Example: Modal Unfolding

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 13 & 14 & 15 & 16 \\ 17 & 18 & 19 & 20 \\ 21 & 22 & 23 & 24 \end{bmatrix}$$

$$\mathcal{A}_{(1)} = \begin{bmatrix} 1 & 2 & 3 & 4 & 13 & 14 & 15 & 16 \\ 5 & 6 & 7 & 8 & 17 & 18 & 19 & 20 \\ 9 & 10 & 11 & 12 & 21 & 22 & 23 & 24 \end{bmatrix}$$

Modal Operations

- Modal Operations take Tensors to Matrices

Example: Modal Unfolding

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 13 & 14 & 15 & 16 \\ 17 & 18 & 19 & 20 \\ 21 & 22 & 23 & 24 \end{bmatrix}$$

$$\mathcal{A}_{(2)} = \begin{bmatrix} 1 & 5 & 9 & 13 & 17 & 21 \\ 2 & 6 & 10 & 14 & 18 & 22 \\ 3 & 7 & 11 & 15 & 19 & 23 \\ 4 & 8 & 12 & 16 & 20 & 24 \end{bmatrix}$$

Modal Operations

- Modal Operations take Tensors to Matrices

Example: Modal Unfolding

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 13 & 14 & 15 & 16 \\ 17 & 18 & 19 & 20 \\ 21 & 22 & 23 & 24 \end{bmatrix}$$

$$\mathcal{A}_{(3)} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 & 17 & 18 & 19 & 20 & 21 & 22 & 23 & 24 \end{bmatrix}$$

Modal Operations

- Modal Operations take Tensors to Matrices
- Modal Unfolding Example

Definition: Modal Product

The **modal product**, denoted $\times_k$, of a 3rd-order tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$ and a matrix $\mathbf{U} \in \mathbb{R}^{J \times n_k}$, where J is any integer, is the product of modal unfolding $\mathcal{A}_{(k)}$ with $\mathbf{U}$. Such that

$$\mathbf{B} = \mathbf{U}\mathcal{A}_{(k)} = \mathcal{A} \times_k \mathbf{U}$$

Modal Product

- Modal Operations take Tensors to Matrices
- Modal Unfolding Example
- Modal Product $A \times_1 \mathbf{U} = \mathbf{U}A_{(1)}$

Example: Modal Product

Modal Product

- Modal Operations take Tensors to Matrices
- Modal Unfolding Example
- Modal Product $A \times_1 \mathbf{U} = \mathbf{U}A_{(1)}$

Example: Modal Product

$$= \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 & 4 & 13 & 14 & 15 & 16 \\ 5 & 6 & 7 & 8 & 17 & 18 & 19 & 20 \\ 9 & 10 & 11 & 12 & 21 & 22 & 23 & 24 \end{bmatrix}$$

Modal Product

- Modal Operations take Tensors to Matrices
- Modal Unfolding Example
- Modal Product $A \times_1 \mathbf{U} = \mathbf{U}A_{(1)}$

Example: Modal Product

$$= \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 & 4 & 13 & 14 & 15 & 16 \\ 5 & 6 & 7 & 8 & 17 & 18 & 19 & 20 \\ 9 & 10 & 11 & 12 & 21 & 22 & 23 & 24 \end{bmatrix}$$

$$= \begin{bmatrix} 5 & 6 & 7 & 8 & 17 & 18 & 19 & 20 \\ -3 & -2 & -1 & 0 & 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 & 25 & 26 & 27 & 28 \end{bmatrix}$$

Higher Order SVD

Definition: HOSVD

Suppose $\mathcal{A}$ is a 3rd-order tensor and $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$. Then there exists a **Higher Order SVD** such that

$$\mathbf{U}_k^T \mathcal{A}_{(k)} = \Sigma_k \mathbf{V}_k^T \quad (1 \leq k \leq d)$$

where $\mathbf{U}_k$ and $\mathbf{V}_k$ are unitary matrices and the matrix Σ_k contains the *singular values* of $\mathcal{A}_{(k)}$ on the *diagonal*, $[\Sigma_k]_{ij}$ where $i = j$, and is zero elsewhere.

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathbf{U}_1^T \mathcal{A}_{(1)} = \hat{\mathcal{A}}_{(1)} \rightarrow \hat{\mathcal{A}}$$
$$\mathbf{U}_2^T \hat{\mathcal{A}}_{(2)} = \hat{\hat{\mathcal{A}}}_{(2)} \rightarrow \hat{\hat{\mathcal{A}}}$$
$$\mathbf{U}_3^T \hat{\hat{\mathcal{A}}}_{(3)} = \mathcal{S}_{(3)} \rightarrow \mathcal{S}$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathcal{S}_1 = \begin{bmatrix} -69.627 & 0.0914 & -1.1 \times 10^{-14} & 3.1 \times 10^{-16} \\ -0.033 & -1.0453 & 2.2 \times 10^{-15} & -7.0 \times 10^{-16} \\ 7.5 \times 10^{-15} & 1.9 \times 10^{-15} & -4.9 \times 10^{-16} & -2.6 \times 10^{-16} \end{bmatrix}$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathcal{S}_1 = \begin{bmatrix} -69.627 & 0.0914 & -1.1\times10^{-14} & 3.1\times10^{-16} \\ -0.033 & -1.0453 & 2.2\times10^{-15} & -7.0\times10^{-16} \\ 7.5\times10^{-15} & 1.9\times10^{-15} & -4.9\times10^{-16} & -2.6\times10^{-16} \end{bmatrix}$$

$$\mathcal{S}_2 = \begin{bmatrix} 0.0201 & 2.212 & -2.8\times10^{-15} & 8.3\times10^{-16} \\ -6.723 & -0.935 & -4.2\times10^{-16} & 9.8\times10^{-16} \\ 5.2\times10^{-15} & -3.9\times10^{-16} & 3.2\times10^{-16} & 8.8\times10^{-16} \end{bmatrix}$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\hat{\mathbf{U}}_1 \mathcal{S}_{(1)} = \hat{\mathcal{S}}_{(1)} \rightarrow \hat{\mathcal{S}}$$
$$\hat{\mathbf{U}}_2 \hat{\mathcal{S}}_{(2)} = \hat{\hat{\mathcal{S}}}_{(2)} \rightarrow \hat{\hat{\mathcal{S}}}$$
$$\hat{\mathbf{U}}_3 \hat{\hat{\mathcal{S}}}_{(3)} = \mathcal{A}_{(3)} \rightarrow \mathcal{A}$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathcal{A}_1 = \begin{bmatrix} 1.0 & 2.0 \\ 5.0 & 6.0 \end{bmatrix}$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathcal{A}_1 = \begin{bmatrix} 1.0 & 2.0 \\ 5.0 & 6.0 \end{bmatrix}$$

$$\mathcal{A}_2 = \begin{bmatrix} 13.0 & 14.0 \\ 17.0 & 18.0 \end{bmatrix}$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathcal{A}_1 = \begin{bmatrix} 1.0 & 2.0 \\ 5.0 & 6.0 \end{bmatrix}$$

$$\mathcal{A}_2 = \begin{bmatrix} 13.0 & 14.0 \\ 17.0 & 18.0 \end{bmatrix}$$

$$\mathcal{S} = \mathcal{A} \times_1 U_1^T \times_2 U_2^T \times_3 U_3^T$$

- Higher Order SVD Definition

Example: 3rd-Order SVD

$$\mathcal{A}_1 = \begin{bmatrix} 1.0 & 2.0 \\ 5.0 & 6.0 \end{bmatrix}$$

$$\mathcal{A}_2 = \begin{bmatrix} 13.0 & 14.0 \\ 17.0 & 18.0 \end{bmatrix}$$

$$\mathcal{S} = \mathcal{A} \times_1 U_1^T \times_2 U_2^T \times_3 U_3^T$$

$$\mathcal{A} = \mathcal{S} \times_1 U_1 \times_2 U_2 \times_3 U_3$$

CP Decomposition

Definition: Rank of a Tensor

The **rank** of a tensor $\mathcal{A}$ is the smallest number of rank 1 tensors that sum to $\mathcal{A}$.

CP Decomposition

Definition: CP Decomposition

A **CP decomposition** of a 3rd-order tensor, $\mathcal{A}$, is defined as a sum of vector outer products, denoted $\circ$, that equal or approximately equal $\mathcal{A}$. For $R = rank(\mathcal{A})$

$$\mathcal{A} = \sum_{r=1}^{R} a_r \circ b_r \circ c_r$$

and for $R < rank(\mathcal{A})$

$$\mathcal{A} \approx \sum_{r=1}^{R} a_r \circ b_r \circ c_r$$

CP Decomposition

Example: CP Decomposition

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

CP Decomposition

Example: CP Decomposition

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

The rank decomposition over $\mathbb{R}$ is $\mathcal{A} = [[\mathbf{A}, \mathbf{B}, \mathbf{C}]]$, where

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \end{bmatrix} \mathbf{B} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \mathbf{C} = \begin{bmatrix} 1 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix}$$

CP Decomposition

Example: CP Decomposition

$$\mathcal{A}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathcal{A}_2 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

The rank decomposition over $\mathbb{R}$ is $\mathcal{A} = [[\mathbf{A}, \mathbf{B}, \mathbf{C}]]$, where

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \end{bmatrix} \mathbf{B} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \mathbf{C} = \begin{bmatrix} 1 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix}$$

but over $\mathbb{C}$

$$\mathbf{A} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix} \mathbf{B} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \mathbf{C} = \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix}$$

Table of Contents

The Problem

The Problem

We have a $3 \times 3 \times 3$ hyperpolarizability tensor and need to rotate it about 3 axes in space and there is currently no known 3rd-order rotation tensor.

The Problem

The Problem

We have a $3 \times 3 \times 3$ hyperpolarizability tensor and need to rotate it about 3 axes in space and there is currently no known 3rd-order rotation tensor.

For matrices and vectors we have rotation matrices that will rotate our matrix/vector around 3 axes:

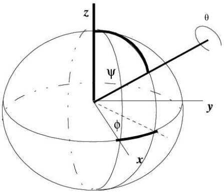
$$R = \begin{bmatrix} \cos(\phi)\cos(\psi) - \cos(\theta)\sin(\phi)\sin(\psi) & -\cos(\theta)\cos(\psi)\sin(\phi) - \cos(\phi)\sin(\psi) & \sin(\theta)\sin(\phi) \\ \cos(\psi)\sin(\phi) + \cos(\theta)\cos(\phi)\sin(\psi) & \cos(\theta)\cos(\phi)\cos(\psi) - \sin(\phi)\sin(\psi) & -\cos(\phi)\sin(\theta) \\ \sin(\theta)\sin(\psi) & \cos(\psi)\sin(\theta) & \cos(\theta) \end{bmatrix}$$

The Problem

The Problem

We have a $3 \times 3 \times 3$ hyperpolarizability tensor and need to rotate it about 3 axes in space and there is currently no known 3rd-order rotation tensor.

For matrices and vectors we have rotation matrices that will rotate our matrix/vector around 3 axes:



The Problem

The Problem

We have a $3 \times 3 \times 3$ hyperpolarizability tensor and need to rotate it about 3 axes in space and there is currently no known 3rd-order rotation tensor.

Rotation by CP Decomposition

$$\mathcal{X} \rightarrow \mathcal{X}_{rot}$$

The Problem

The Problem

We have a $3 \times 3 \times 3$ hyperpolarizability tensor and need to rotate it about 3 axes in space and there is currently no known 3rd-order rotation tensor.

Rotation by CP Decomposition

$$\mathcal{X} \to \mathcal{X}_{rot}$$

$$\mathcal{X} = \sum_{j=1}^{3} (a_j) \circ (b_j) \circ (c_j)$$

The Problem

The Problem

We have a $3 \times 3 \times 3$ hyperpolarizability tensor and need to rotate it about 3 axes in space and there is currently no known 3rd-order rotation tensor.

Rotation by CP Decomposition

$$\mathcal{X} \to \mathcal{X}_{rot}$$

$$\mathcal{X} = \sum_{j=1}^{3} (a_j) \circ (b_j) \circ (c_j)$$

$$\mathcal{X}_{rot} = \sum_{j=1}^{3} (Ra_j) \circ (Rb_j) \circ (Rc_j)$$

The Problem

Rotation by CP Decomposition

$$\mathcal{X} \to \mathcal{X}_{rot}$$

$$\mathcal{X} = \sum_{j=1}^{3} (a_j) \circ (b_j) \circ (c_j)$$

$$\mathcal{X}_{rot} = \sum_{j=1}^{3} (Ra_j) \circ (Rb_j) \circ (Rc_j)$$

The Problem

Rotation by CP Decomposition

$$\mathcal{X} \to \mathcal{X}_{rot}$$

$$\mathcal{X} = \sum_{j=1}^{3} (a_j) \circ (b_j) \circ (c_j)$$

$$\mathcal{X}_{rot} = \sum_{j=1}^{3} (Ra_j) \circ (Rb_j) \circ (Rc_j)$$

$$= [Ra_1|Ra_2|Ra_3] \odot [Rb_1|Rb_2|Rb_3] \odot [Rc_1|Rc_2|Rc_3]$$

The Problem

Rotation by CP Decomposition

$$\mathcal{X} \to \mathcal{X}_{rot}$$

$$\mathcal{X} = \sum_{j=1}^{3} (a_j) \circ (b_j) \circ (c_j)$$

$$\begin{aligned}\mathcal{X}_{rot} &= \sum_{j=1}^{3} (Ra_j) \circ (Rb_j) \circ (Rc_j) \\ &= [Ra_1|Ra_2|Ra_3] \odot [Rb_1|Rb_2|Rb_3] \odot [Rc_1|Rc_2|Rc_3] \\ &= R[a_1|a_2|a_3] \odot R[b_1|b_2|b_3] \odot R[c_1|c_2|c_3]\end{aligned}$$

The Problem

Rotation by CP Decomposition

$$\mathcal{X} \to \mathcal{X}_{rot}$$

$$\mathcal{X} = \sum_{j=1}^{3} (a_j) \circ (b_j) \circ (c_j)$$

$$\begin{aligned}\mathcal{X}_{rot} &= \sum_{j=1}^{3} (Ra_j) \circ (Rb_j) \circ (Rc_j) \\ &= [Ra_1|Ra_2|Ra_3] \odot [Rb_1|Rb_2|Rb_3] \odot [Rc_1|Rc_2|Rc_3] \\ &= R[a_1|a_2|a_3] \odot R[b_1|b_2|b_3] \odot R[c_1|c_2|c_3] \\ &= R\mathbf{A} \odot R\mathbf{B} \odot R\mathbf{C}\end{aligned}$$

Table of Contents

The End

1. G.H. Golub and C.F. Van Loan, *Matrix Computations*, (The Johns Hopkins University Press 2013).
2. Hongfei Wang et al, "Quantitative spectral and orientational analysis in surface sum frequency generation vibrational spectroscopy (SFG-VS)", International Reviews in Physical Chemistry (2005), (24) no. 2, 191-256.
3. Kolda, T.G. and Bader, B.W., "Tensor Decompositions and Applications", SIAM Review (2009), (51) no. 3, 455-500.
4. Carroll, J.Douglas and Chang, Jih-Jie, "Analysis of individual differences in multidimensional scaling via an n-way generalization of Eckart-Young decomposition", Psychometrika (1970), (35) no. 3, 283-319.

The End

1. P. Paatero, “A weighted non-negative least squares algorithm for three-way PARAFAC factor analysis”, Chemometrics and Intelligent Laboratory Systems (1997), (38) no. 2, 223-242.
2. N. K. M. Faber and R. Bro, and P. K. Hopke, “Recent developments in CANDECOMP/PARAFAC algorithms: A critical review”, Chemometrics and Intelligent Laboratory Systems (2003), (65), 119-137.
3. J. B. Kruskal, “Rank, decomposition, and uniqueness for 3-way and N-way arrays, in Multiway Data Analysis”, 7-18.