Multi-linear Algebra - Tensor Ranks & CP decomposition Lecture 15

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Matrix rank

Recall:

A matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ is of rank r if and only if:

- There are exactly r linearly independent columns in ${\bf A}$
- There are exactly r linearly independent row in \mathbf{A}
- The image of the linear map induced by **A** is of dimension r
- r is the smallest number such that exist $\mathbf{u}_i \in \mathbb{R}^m$ and $\mathbf{v}_i \in \mathbb{R}^n$ and real numbers $\sigma_i > 0$ such that

$$\mathbf{A} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\top} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i$$

• r is the smallest number, such that there exist r-dimensional subspaces $V \subseteq \mathbb{R}^m$ and $U \subseteq \mathbb{R}^n$, such that A is an element of the induced tensor space $V \otimes U \subseteq \mathbb{R}^{m \times n}$

Canonical Polyadic (CP) Decomposition

Definition:

Let $\mathbf{X} \in \mathbb{R}^{n_1 \times ... \times n_d}$ be a tensor of order d. A representation of \mathbf{X} as a sum of elementary tensors

$$\mathbf{X} = \sum_{p=1}^{r} \mathbf{v}_{1,p} \otimes ... \otimes \mathbf{v}_{d,p} = \sum_{p=1}^{r} \bigotimes_{i=1}^{d} \mathbf{v}_{i,p}$$

for $\mathbf{v}_{i,p} \in \mathbb{R}^{n_i}$ is called a canonical polyadic (CP) representation of \mathbf{X} . The number of terms r is called the "rank of the representation". The minimal r, such that there exists a CP decomposition of X with rank r, is called the canonical rank or CP-rank of \mathbf{X} .

$$\begin{bmatrix} \begin{bmatrix} 1.5 & -2.5 \\ 2.5 & -2.5 \end{bmatrix}, \begin{bmatrix} -2 & 2 \\ -2 & 2 \end{bmatrix} \end{bmatrix}$$

¹J. Håstad, Journal of Algorithms, 1990

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$$= 2 \begin{bmatrix} 1 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ -1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ -1 \end{bmatrix} + (-.5) \begin{bmatrix} 1 \\ -1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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The rank of this decomposition is 2 However, we also find

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The rank of this decomposition is 8.

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Deciding whether a rational tensor has CP-rank r is NP-hard ¹

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CP deocposition

Given a tensor \mathbf{X} , we seek to find

$$\mathbf{X}_* = \underset{\text{CP-rank}(\mathbf{X}_r) \le r}{\operatorname{argmin}} \|\mathbf{X} - \mathbf{X}_r\| \tag{1}$$

Matrices:

• Eckart–Young gives insight for unitarily invariant matrices

Tensors

• For many tensor ranks $r \geq 2$ and all orders $d \geq 3$, regardless of the choice of $\|\cdot\|$:

Eq.
$$(??)$$
 is ill-defined²!

- There are methods calculating approximate CP decompositions of higher-order tensors
 - \rightarrow Challenging and expensive task
 - \rightarrow In practice approached using optimization algorithms

²De Silva & Lim, SIAM Journal on Matrix Analysis and Applications, 2008

Set of Tensors with Fixed Canonical Rank

Ill-Definedness of Eq. (??) can be connected to the following problem:

Let's consider

$$\mathcal{M}_{\leq r} = \left\{ \mathbf{X} \in \mathbb{R}^{n_1 \times \dots \times n_d} \mid \mathrm{CP} - \mathrm{rank}(\mathbf{X}) \leq r \right\}$$

the sequence

$$\mathbf{X}_n = n\left(\mathbf{u} + \frac{1}{n}\mathbf{v}\right) \otimes \left(\mathbf{u} + \frac{1}{n}\mathbf{v}\right) \otimes \left(\mathbf{u} + \frac{1}{n}\mathbf{v}\right) \otimes -n\mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u}$$

with $\mathbf{u}, \mathbf{v} \in \mathbb{R}^m$, $\|\mathbf{v}\| = \|\mathbf{u}\| = 1$ and $\langle \mathbf{v}, \mathbf{u} \rangle \neq 1$.

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Note that $\mathbf{X}_n \in \mathcal{M}_{\leq r}$ for all $n \in \mathbb{N}$, however

$$\lim_{n\to\infty} \mathbf{X}_n = \mathbf{v} \otimes \mathbf{u} \otimes \mathbf{u} + \mathbf{u} \otimes \mathbf{v} \otimes \mathbf{u} + \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{v} \notin \mathcal{M}_{\leq r}$$

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Similarly

$$\mathcal{M}_r = \{ \mathbf{X} \in \mathbb{R}^{n_1 \times \dots \times n_d} \mid \text{CP} - \text{rank}(\mathbf{X}) = r \}$$

is not closed.

Difficulties CP format

- CP decomposition sets have very little structure
- Low-rank matrices for manifolds
 - \rightarrow we can use optimization techniques on Manifolds
- \bullet CP rank tensor do not form any kind of manifold \to optimization on such sets is extremely difficult
- The approximation is ambiguous
 - \rightarrow Many parameters $\mathbf{v}_{p,i}$ approximate the same tensor equally well
 - ⇒ More in Mitchell & Burdick, Journal of Chemometrics, 1994

The CP format allows an unparalleled complexity reduction for tensors with small canonical rank!

Computational Aspects of CP decomposition

Recall:

Storing a tensor $\mathbf{X} \in \mathbb{R}^{n_1 \times ... \times n_d}$ requires $\mathcal{O}(n^d)$, where $n = \max_i n_i$.

Computational Aspects of CP decomposition

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In the CP format, we store the vector entries $\mathbf{v}_{i,p}$.

- \rightarrow requires $\mathcal{O}(ndr)$
- \rightarrow linearly in the dimension

What about operations?

Addition in CP format

Consider

Then the addition of **X** and $\bar{\mathbf{X}}$ i.e.,

$$\mathbf{X} + \bar{\mathbf{X}} = \sum_{p=1}^{r} \bigotimes_{i=1}^{d} \mathbf{v}_{i,p} + \sum_{p=1}^{\bar{r}} \bigotimes_{i=1}^{d} \bar{\mathbf{v}}_{i,p} = \sum_{p=1}^{\bar{r}+r} \bigotimes_{i=1}^{d} \mathbf{W}_{i,p}$$

with

$$\mathbf{w}_{i,p} = \left\{ \mathbf{v}_{i,p} \quad k \le r \bar{\mathbf{v}}_{i,p} \quad k > r \right. \tag{2}$$

In order to access the element, we have to perform the following operation

$$(\mathbf{X} + \bar{\mathbf{X}})[i_1, ..., i_d] = \left(\sum_{p=1}^{\bar{r}+r} \bigotimes_{k=1}^{d} \mathbf{W}_{i,p}\right)[i_1, ..., i_d] = \sum_{p=1}^{\bar{r}+r} \prod_{k=1}^{d} \mathbf{W}_{i,p}[i_k]$$

Which scales as $\mathcal{O}(nd(\bar{r}+r))$, compared to adding two dense tensors $\mathcal{O}(n^d)$

kth-mode contraction

Given a matrix $\mathbf{A} \in \mathbb{R}^{n_k \times m}$. Then

$$\mathbf{X} *_{k} \mathbf{A} = \left(\sum_{p=1}^{\bar{r}+r} \bigotimes_{k=1}^{d} \mathbf{W}_{i,p}\right) *_{k} \mathbf{A}$$

$$= \sum_{p=1}^{\bar{r}+r} \left(\bigotimes_{k=1}^{d} \mathbf{W}_{i,p}\right) *_{k} \mathbf{A}$$

$$= \sum_{p=1}^{\bar{r}+r} \mathbf{v}_{1,p} \otimes ... \otimes \left(\mathbf{A}^{\top} \mathbf{v}_{k,p}\right) \otimes ... \otimes \mathbf{v}_{d,p}$$

Other tensor operations in CP format

Operation	CP-Format	dense tensor
Hadamard Product	$\mathcal{O}(ndrar{r})$	$\mathcal{O}(n^d)$
Frobenius Inner Product	$\mathcal{O}(ndrar{r})$	$\mathcal{O}(n^d)$
Frobenius Norm	$\mathcal{O}(ndr^2)$	$\mathcal{O}(n^d)$
k-mode product	$\mathcal{O}((d+m)nr)$	$\mathcal{O}(n^d m)$