Multi-linear Algebra
– Tensor Train Decomposition –
Lecture 18

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29/03/2024

Recall

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- CP decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \ldots \times n_d}$. Then

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

Storage of CP format:
CP rank:

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Storage of CP format: $\mathcal{O}(rnd)$
CP rank: minimal r s.t. we can express $\mathbf{A}$ in the above format

Recall

- Tucker decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \ldots \times n_d}$. Then

$$\begin{aligned}\mathbf{A} &= \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} \mathbf{C}[i_1, ..., i_d] \cdot \mathbf{u}_{1,i_1} \otimes \mathbf{u}_{2,i_2} \otimes \cdots \otimes \mathbf{u}_{d,i_1} \\ &= \mathbf{C} *_1 \mathbf{U}_1 *_2 \mathbf{U}_2 ... *_d \mathbf{U}_d\end{aligned}$$

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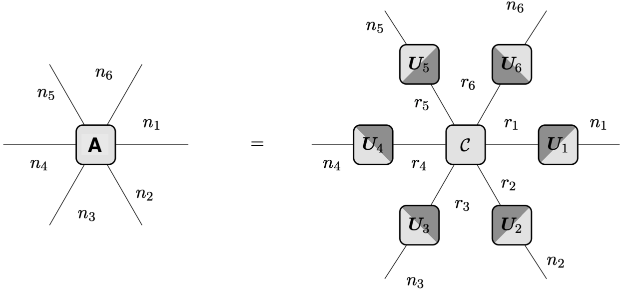

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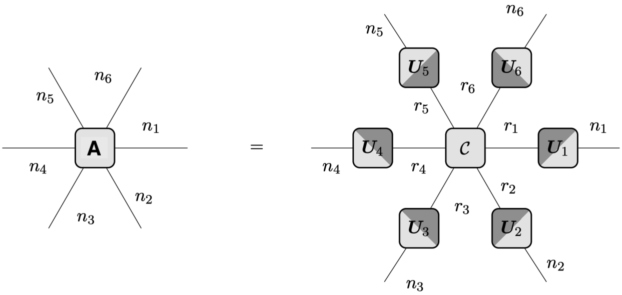

Storage of Tucker format: $\mathcal{O}(r^d + rnd)$
T-rank: $\mathbf{r} = (r_1, \ldots, r_d)$
Advantage:

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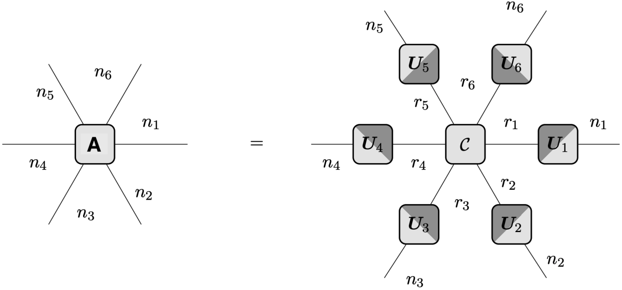

Storage of Tucker format: $\mathcal{O}(r^d + rnd)$
Advantage:

1. Can be computed using HOSVD
2. Closed set of low-rank tensors
3. Manifold structure on the set of tensors with fixed rank
4. Can be sketched

Sketching Tucker

Compute a low-Tucker rank approximation using:

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The computational complexity of the most common operations scales linearly in the order if all operands are given in TT representation

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The computational complexity of the most common operations scales linearly in the order if all operands are given in TT representation

$\Rightarrow$ TT decomposition unifies advantages of CP and Tucker

TT decomposition – A tail of subspaces!

Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \ldots \times n_d}$ be our target tensor

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$$U_1 \subseteq \mathbb{R}^{n_1},\ U_2 \subseteq \mathbb{R}^{n_1 \times n_2},\ \ldots,\ U_{d-1} \subseteq \mathbb{R}^{n_1 \times \ldots \times n_{d-1}}$$

s.t. the final subspace contains the target tensor:

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&U_3 \subseteq U_2 \otimes \mathbb{R}^{n_3} \subseteq \mathbb{R}^{n_1 \times n_2 \times n_3} && \text{with } \mathbf{A} \in U_3 \otimes \mathbb{R}^{n_4 \times \ldots \times n_d}
\end{aligned}$$

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&\quad\vdots && \quad\vdots \\
&U_{d-1} \subseteq U_{d-2} \otimes \mathbb{R}^{n_{d-1}} \subseteq \mathbb{R}^{n_1 \times \ldots \times n_{d-1}} && \text{with } \mathbf{A} \in U_{d-1} \otimes \mathbb{R}^{n_d}
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- Note that $U_k \subseteq U_{k-1} \otimes \mathbb{R}^{n_k} \subseteq \mathbb{R}^{n_1 \times ... \times n_k}$ ensures that

$$\mathbf{V}_{k,j} = \sum_{i=1}^{r_{k-1}} \mathbf{V}_{k-1,i} \otimes \mathbf{u}_{k,i,j}$$

for some $\mathbf{u}_{k,i,j} \in \mathbb{R}^{n_k}$.

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- Writing the (orthogonal) basis as a tensor

$$\mathbf{W}_k[i_1, ..., i_k, j] = \mathbf{V}_{k,j}[i_1, ..., i_k]$$

  and defining

$$\mathbf{U}_k[i, \ell, j] = \mathbf{u}_{k,i,j}[\ell]$$

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  with $\mathbf{W} \in \mathbb{R}^{n_1 \times ... \times n_k \times r_k}$ and $\mathbf{U}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$

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&= \sum_{i=1}^{r_{k-1}} \mathbf{V}_{k-1,i}[i_1, ..., i_{k-1}] \mathbf{u}_{k,i,j}[i_k] \\
&= \sum_{i=1}^{r_{k-1}} \mathbf{W}_{k-1}[i_1, ..., i_{k-1}, i] \mathbf{U}_k[i, i_k, j]
\end{aligned}$$

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&= \left(\mathbf{W}_{k-1} *_{(k),(1)} \mathbf{U}_k \right) [i_1, ..., i_{k-1}, i_k, j]
\end{aligned}$$

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So, recursively applied, this yields

$$\mathbf{A} = \mathbf{W}_{d-1} *_{(d),(1)} \mathbf{U}_d$$

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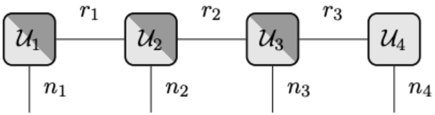
\end{aligned}
$$

Or as a diagram



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$$= (\mathbf{U}_1)^{n_1}_{r_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)^{r_1}_{n_2\cdots n_d} \qquad \text{SVD}$$

TT-SVD (another variant of HOSVD)

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\end{aligned}
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TT-SVD (another variant of HOSVD)

$\mathbf{A}_{n_1,\ldots,n_d}$	
$= \mathbf{A}^{n_1}_{n_2\cdots n_d}$	reshape to $n_1 \times \prod_{j\neq i} n_j$
$= (\mathbf{U}_1)^{n_1}_{r_1}\,(\boldsymbol{\Sigma}_1\mathbf{V}_1^\top)^{r_1}_{n_2\cdots n_d}$	SVD
$= (\mathbf{U}_1)^{n_1}_{r_1}\,(\boldsymbol{\Sigma}_1\mathbf{V}_1^\top)^{r_1\cdot n_2}_{n_3\cdots n_d}$	reshape of $(\boldsymbol{\Sigma}_1\mathbf{V}_1^\top)$
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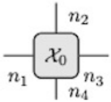
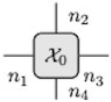
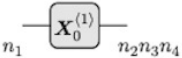
&= (\mathbf{U}_1)^{n_1}_{r_1}\,(\mathbf{U}_2)^{r_1\cdot n_2}_{r_2}\,(\mathbf{U}_3)^{r_2\cdot n_3}_{r_3}\,(\mathbf{\Sigma}_3\mathbf{V}_3^\top)^{r_3}_{n_4\cdots n_d} && \text{SVD of } (\mathbf{\Sigma}_2\mathbf{V}_2^\top) \\
&\ \vdots \\
&= \underbrace{(\mathbf{U}_1)^{n_1}_{r_1}}_{\mathbf{U}_1[n_d]}\cdots\underbrace{(\mathbf{U}_{d-1})^{r_{d-2}\cdot n_{d-1}}_{r_{d-1}}}_{=:\mathbf{U}_{d-1}[n_{d-1}]}\underbrace{(\mathbf{\Sigma}_{d-1}\mathbf{V}_{d-1}^\top)^{r_{d-1}}_{n_d}}_{=:\mathbf{U}_d[n_d]}
\end{aligned}
$$

TT-SVD (diagrammatically)

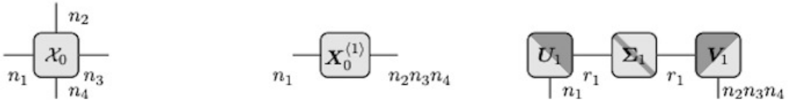


TT-SVD (diagrammatically)

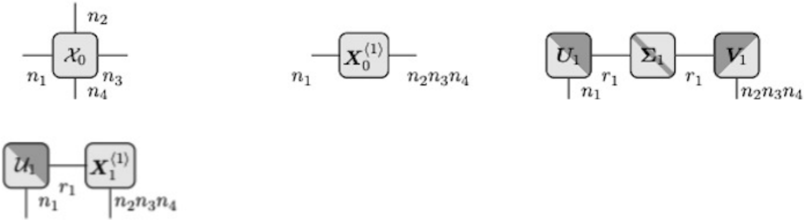




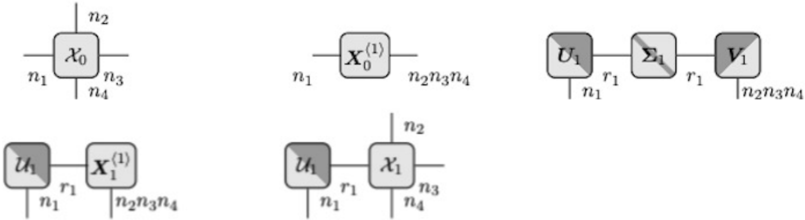
TT-SVD (diagrammatically)



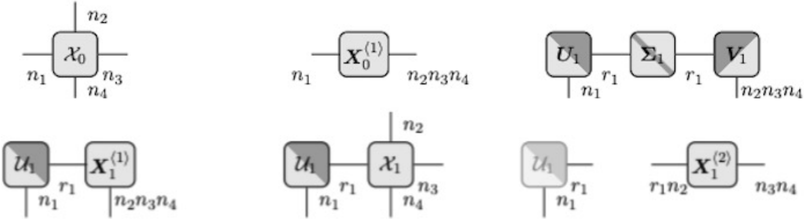
TT-SVD (diagrammatically)



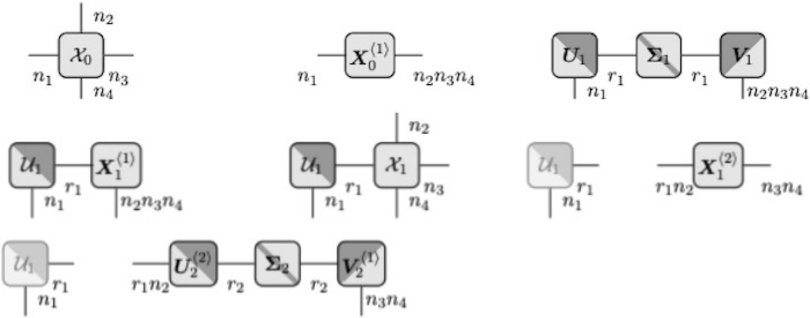
TT-SVD (diagrammatically)



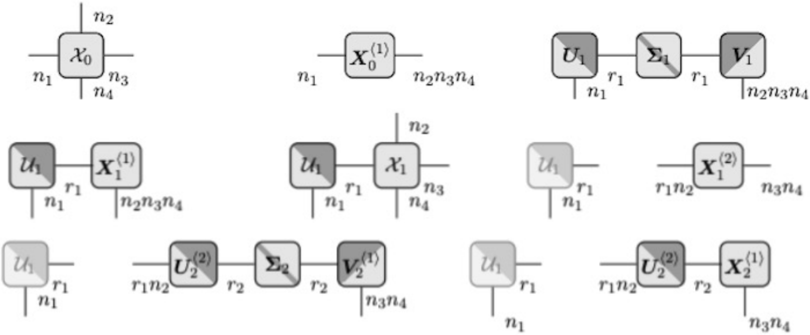
TT-SVD (diagrammatically)



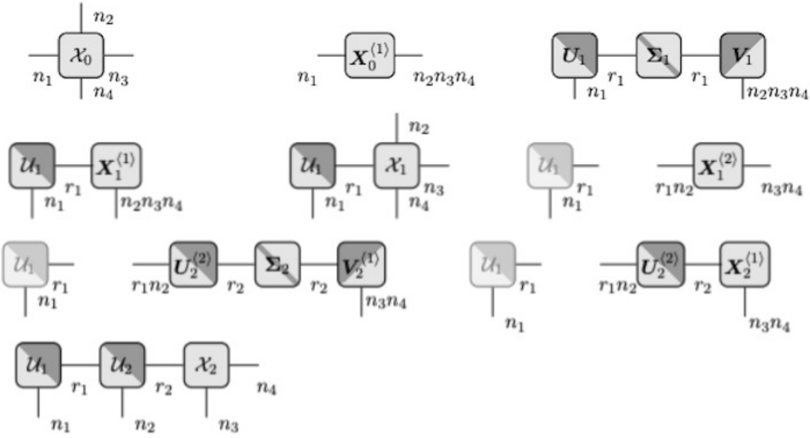
TT-SVD (diagrammatically)



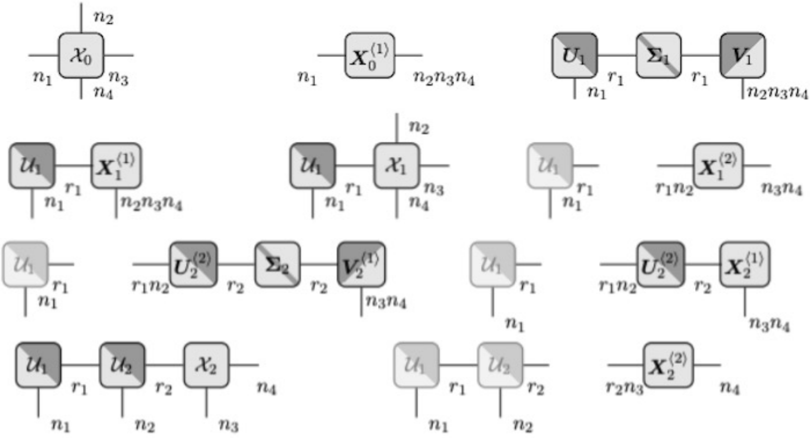
TT-SVD (diagrammatically)



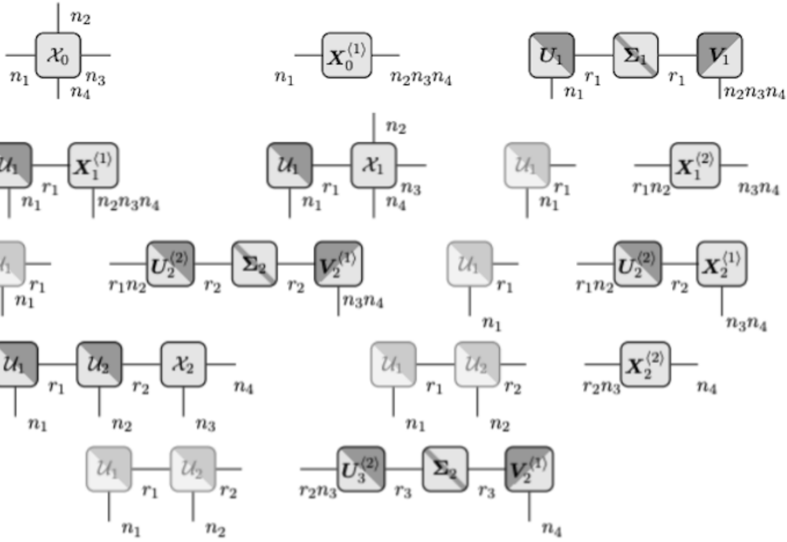
TT-SVD (diagrammatically)



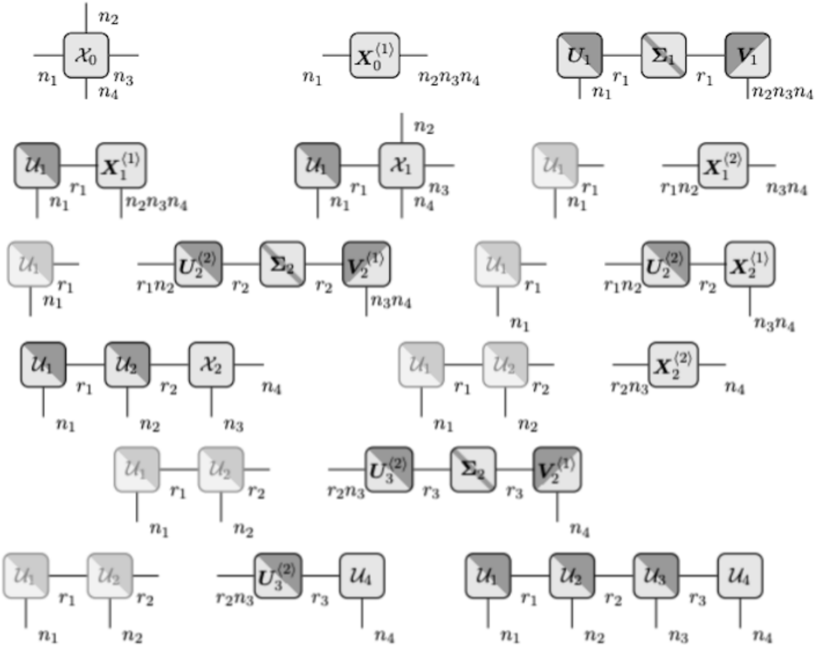
TT-SVD (diagrammatically)



TT-SVD (diagrammatically)



TT-SVD (diagrammatically)



TT Pseudo-code

We introduce the notation

$$\mathbf{A}^{\langle k \rangle} = \mathrm{MAT}_{(1,\ldots,k)}(\mathbf{A})$$

for the matricization that flattens the first k and the last $d-k$ modes

Algorithm:

Input: Target tensor $\mathbf{A}$, target rank $(r_1, \ldots, r_d)$
Output: Component tensors $\mathbf{U}_i \in \mathbb{R}^{r_{i-1} \times n_i \times r_i}$

$\mathbf{A}_1 = \mathbf{A}^{\langle 1 \rangle}$
$\tilde{\mathbf{U}}_1,\ \mathbf{\Sigma}_1,\ \mathbf{V}_1 = \mathrm{SVD}(\mathbf{A}_1, r_1)$
$\mathbf{U}_1 = \mathrm{unfild}(\tilde{\mathbf{U}}_1)$ — special treatment for 1^{st} mode
$\mathcal{V}_1 = \mathrm{unfold}(\mathbf{\Sigma}_1 \mathbf{V}_1^\top)$
$A_2 = \mathcal{V}_1^{\langle 2 \rangle}$
for $k = 2 : d-1$
    $\tilde{\mathbf{U}}_k,\ \mathbf{\Sigma}_k,\ \mathbf{V}_k = \mathrm{SVD}(\mathbf{A}_k, r_k)$
    $\mathbf{U}_k = \mathrm{unfold}(\tilde{\mathbf{U}}_k)$
    $\mathcal{V}_k = \mathrm{unfold}(\mathbf{\Sigma}_k \mathbf{V}_k^\top)$
    $A_{k+1} = \mathcal{V}_k^{\langle 2 \rangle}$
$\tilde{\mathbf{U}}_d = \mathcal{V}_{d-1}$
$\mathbf{U}_d = \mathrm{unfold}(\tilde{\mathbf{U}}_d)$ — special treatment for d^{th} mode

TT decomposition

Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \ldots \times n_d}$. We call a factorization

$$\mathbf{A}[i_1, ..., i_d] = \mathbf{U}_1[i_1]\mathbf{U}_2[i_2] \cdots \mathbf{U}_d[i_d]$$

a TT representation of $\mathbf{A}$.

Note: This reveals the alternative name Matrix-product-states

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Storing in TT format scales as

$$\mathcal{O}(r^2 dn)$$

Accessing Entries

Let consider $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4}$.Then

$$\mathbf{A}[i_1, ..., i_4] = \sum_{k_3=1}^{r_3} \sum_{k_2=1}^{r_2} \sum_{k_1=1}^{r_1} \mathbf{U}_1[1, i_1, k_1]\mathbf{U}_2[k_1, i_2, k_2]\mathbf{U}_3[k_2, i_3, k_3]\mathbf{U}_4[k_3, i_4, 1]$$

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Let consider $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4}$.Then

$$\begin{aligned}
\mathbf{A}[i_1, ..., i_4] &= \sum_{k_3=1}^{r_3} \sum_{k_2=1}^{r_2} \sum_{k_1=1}^{r_1} \mathbf{U}_1[1, i_1, k_1]\mathbf{U}_2[k_1, i_2, k_2]\mathbf{U}_3[k_2, i_3, k_3]\mathbf{U}_4[k_3, i_4, 1] \\
&= \sum_{k_3=1}^{r_3} \sum_{k_2=1}^{r_2} \underbrace{\left(\sum_{k_1=1}^{r_1} \mathbf{U}_1[1, i_1, k_1]\mathbf{U}_2[k_1, i_2, k_2] \right)}_{\substack{\in \mathcal{O}(r) \text{ for fixed } i_1, i_2, k_2 \\ \in \mathcal{O}(r^2) \text{ since } k_2 \in [\![r_2]\!]}} \mathbf{U}_3[k_2, i_3, k_3]\mathbf{U}_4[k_3, i_4, 1]
\end{aligned}$$

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$$\begin{aligned}
\mathbf{A}[i_1, ..., i_4] &= \sum_{k_3=1}^{r_3} \sum_{k_2=1}^{r_2} \sum_{k_1=1}^{r_1} \mathbf{U}_1[1, i_1, k_1]\mathbf{U}_2[k_1, i_2, k_2]\mathbf{U}_3[k_2, i_3, k_3]\mathbf{U}_4[k_3, i_4, 1] \\
&= \sum_{k_3=1}^{r_3} \sum_{k_2=1}^{r_2} \underbrace{\left(\sum_{k_1=1}^{r_1} \mathbf{U}_1[1, i_1, k_1]\mathbf{U}_2[k_1, i_2, k_2] \right)}_{\substack{\in \mathcal{O}(r) \text{ for fixed } i_1, i_2, k_2 \\ \in \mathcal{O}(r^2) \text{ since } k_2 \in [\![r_2]\!]}} \mathbf{U}_3[k_2, i_3, k_3]\mathbf{U}_4[k_3, i_4, 1] \\
&= \sum_{k_3=1}^{r_3} \underbrace{\left(\sum_{k_2=1}^{r_2} \mathbf{W}_1[1, i_1, i_2, k_2]\mathbf{U}_3[k_2, i_3, k_3] \right)}_{\in \mathcal{O}(r^2)} \mathbf{U}_4[k_3, i_4, 1] \\
&= ...
\end{aligned}$$

Generalizing this idea leads to the computational scaling $\mathcal{O}(dr^2)$

Adding TT decomposition

$$
\begin{aligned}
&(\mathbf{A}+\bar{\mathbf{A}})[i_1,...,i_d] \\
&= \mathbf{U}_{1,i_1}\mathbf{U}_{2,i_2}...\mathbf{U}_{d-1,i_{d-1}}\mathbf{U}_{d,i_d} + \bar{\mathbf{U}}_{1,i_1}\bar{\mathbf{U}}_{2,i_2}...\bar{\mathbf{U}}_{d-1,i_{d-1}}\bar{\mathbf{U}}_{d,i_d} \\
&= \begin{pmatrix}\mathbf{U}_{1,i_1} & \bar{\mathbf{U}}_{1,i_1}\end{pmatrix}\begin{pmatrix}\mathbf{U}_{2,i_2} & \mathbf{0}\\ \mathbf{0} & \bar{\mathbf{U}}_{2,i_2}\end{pmatrix}\cdots\begin{pmatrix}\mathbf{U}_{d-1,i_{d-1}} & \mathbf{0}\\ \mathbf{0} & \bar{\mathbf{U}}_{d-1,i_{d-1}}\end{pmatrix}\begin{pmatrix}\mathbf{U}_{d,i_d}\\ \bar{\mathbf{U}}_{d,i_d}\end{pmatrix} \\
&= \mathbf{W}_{1,i_1}\mathbf{W}_{2,i_2}...\mathbf{W}_{d-1,i_{d-1}}\mathbf{W}_{d,i_d}
\end{aligned}
$$

Which is a valid TT representation of $\mathbf{A}+\bar{\mathbf{A}}$ of rant $\mathbf{r}+\bar{\mathbf{r}}$.
Thus the scaling is

$$\mathcal{O}(d(r+\bar{r})^2)$$

where $r=\max(\mathbf{r})$, and $\bar{r}=\max(\bar{\mathbf{r}})$

Other operations

Operation	TT	Tucker	CP
Had. Prod.	$\mathcal{O}(ndr^2\bar{r}^2)$	$\mathcal{O}(ndr\bar{r} + r^d\bar{r}^d)$	$\mathcal{O}(ndr\bar{r})$
Frob. In. Prod.	$\mathcal{O}(ndr^3)$	$\mathcal{O}(ndr\bar{r} + dr\bar{r}^d + r^d)$	$\mathcal{O}(ndr\bar{r})$
Frob. Norm	$\mathcal{O}(r^2n)$	$\mathcal{O}(r^d)$	$\mathcal{O}(ndr^2)$
k-mode Prod.	$\mathcal{O}(mnr^2)$	$\mathcal{O}(mnr + mr^2 + r^{d+1})$	$\mathcal{O}((d+m)nr)$