Inter-University Research Institute Corporation / Research Organization of Information and Systems
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# Fast Tucker Rank Reduction for Non-Negative Tensors Using Mean-Field Approximation

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github.com/gkazunii/Legendre-tucker-rank-reduction

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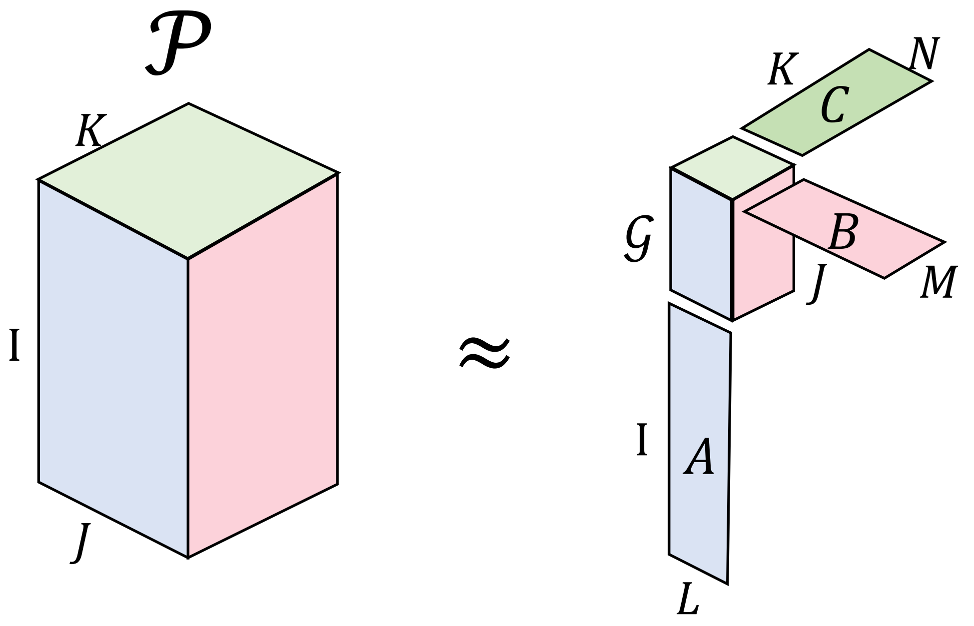
# Tensor low-rank approximation




$$\mathcal{P}_{ijk} = \sum_{l=1}^{L}\sum_{m=1}^{M}\sum_{n=1}^{N} \mathcal{G}_{lmn}\, A_{il}B_{jm}C_{kn}$$

Tucker rank of $\mathcal{P}$ : $(L, M, N)$ $L \leq I, M \leq J, N \leq K$

In this presentation, Tucker rank is simply referred to as Rank.

Rank (1,1,1) is called just rank 1 .

Approximating tensors with low rank tensors reduce memory requirements.

Frobenius error or KL error minimization

Many non-negative low-rank approximation methods are based on a **gradient method**.
→ It requires appropriate settings for **initial values, stopping criterion, and learning rates.** 😢😢

**This study...**

- Maps non-negative tensors to distributions, and derive a formula for **the best rank-1 approximation**
- Understands the rank-1 approximation of a non-negative tensor as a **mean-field approximation**
- Proposes a fast Tucker rank approximation (**LTR**) for nonnegative tensors based on the formula

# Contents

- Best Rank-1 Approximation for Minimizing the KL divergence
  - Make a mapping from a tensor to a distribution
  - A rank-1 condition using parameters of the distribution
  - Rank-1 Approximation as a mean-field approximation
- Legendre Tucker Rank Reduction(LTR)
  - A fast low-rank approximation for non-negative tensors
  - Not based on a gradient method.
- Experiment
- Conclusion

# Introduction of log-linear model on poset

**Poset** $S$ is a poset $\Leftrightarrow$ for all $s_1, s_2, s_3 \in S$ the following three properties are satisfied.

(1) **Reflexivity**: $s_1 \leq s_1$ (2) **Antisymmetry:** $s_1 \leq s_2, s_2 \leq s_1 \Rightarrow s_1 = s_2$ (3) **Transitivity:** $s_1 \leq s_2, s_2 \leq s_3 \Rightarrow s_1 \leq s_3$

## Log-linear model on poset S

We define the log-linear model on a poset S as a mapping $p: S \rightarrow (0,1)$ . **Natural parameters $\boldsymbol{\theta}$** describe the model.

$$p_\theta(x) = \exp\left[\sum_{s \leq x} \theta(s)\right] \quad x \in S$$

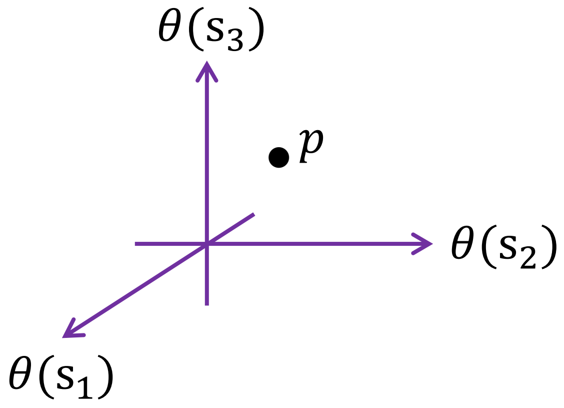
We can also describe the model by **expectation parameters $\eta$** if we use Zeta function.

$$\eta(x) = \sum_{s \geq x} p(s) \qquad p_\eta(x) = \sum_{s \in S} \mu(x,s)\eta(s)$$

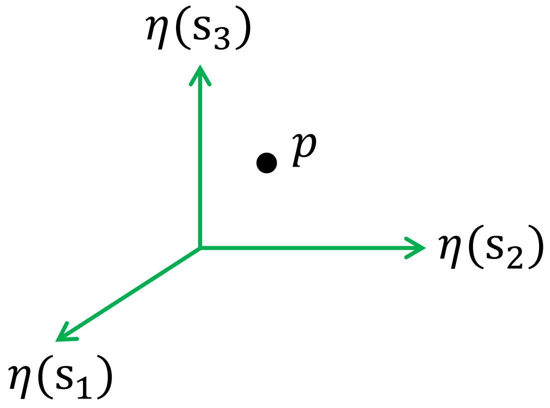
Möbius function

$$\mu(x,s) = \begin{cases} 1 & \text{if } x = y \\ -\sum_{x \leq s < y} \mu(x,s) & \text{if } x < y \\ 0 & \text{otherwise} \end{cases}$$

$\theta$-space




$\eta$-space

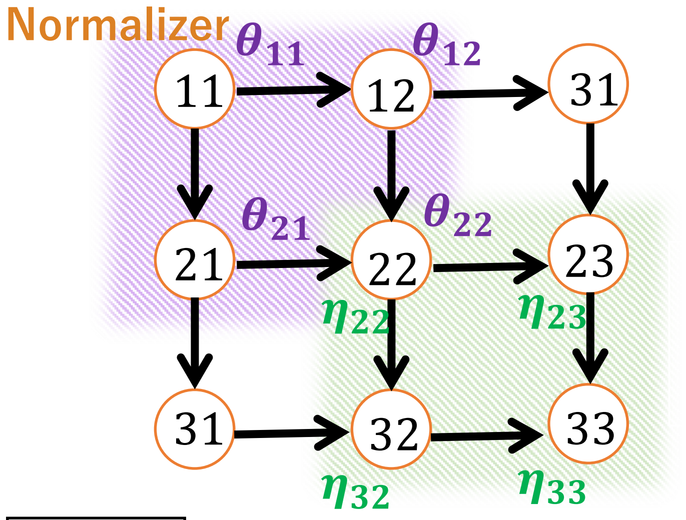



Mahito Sugiyama, Hiroyuki Nakahara and Koji Tsuda "Tensor balancing on statistical manifold"(2017) ICML.

# Mapping a poset to a non-negative matrix/tensor.

## Matrix

$S = \{(i,j) | i,j = \{1,2,\cdots n\}\}$ $\quad (i_1,j_1) \le (i_2,j_2) \Leftrightarrow i_1 \le i_2 \text{ and } j_1 \le j_2$




$$p_\theta(2,2) = \exp[\theta_{11} + \theta_{12} + \theta_{21} + \theta_{22}]$$

$$p_\eta(2,2) = \eta_{22} - \eta_{23} - \eta_{32} + \eta_{33}$$

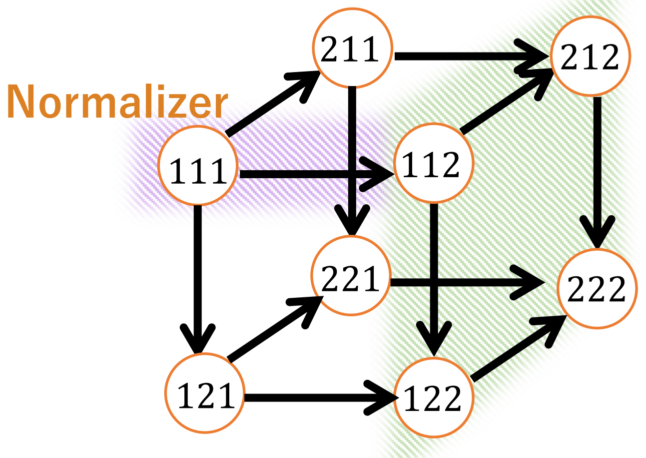
$$p_\theta(i,j) = \exp\left[\sum_{i' \le i} \sum_{j' \le j} \theta_{i'j'}\right]$$

**Relation between distribution and matrix**

Random Variable : index $i, j$
Sample space : index set
Value of the probability : element $P_{ij}$

## Tensor

$S = \{(i,j,k) | i,j,k = \{1,2,\cdots n\}\}$ $\quad (i_1,j_1,k_1) \le (i_2,j_2,k_2) \Leftrightarrow i_1 \le i_2 \text{ and } j_1 \le j_2 \text{ and } k_1 \le k_2$




$$p_\theta(1,1,2) = \exp[\theta_{111} + \theta_{112}]$$

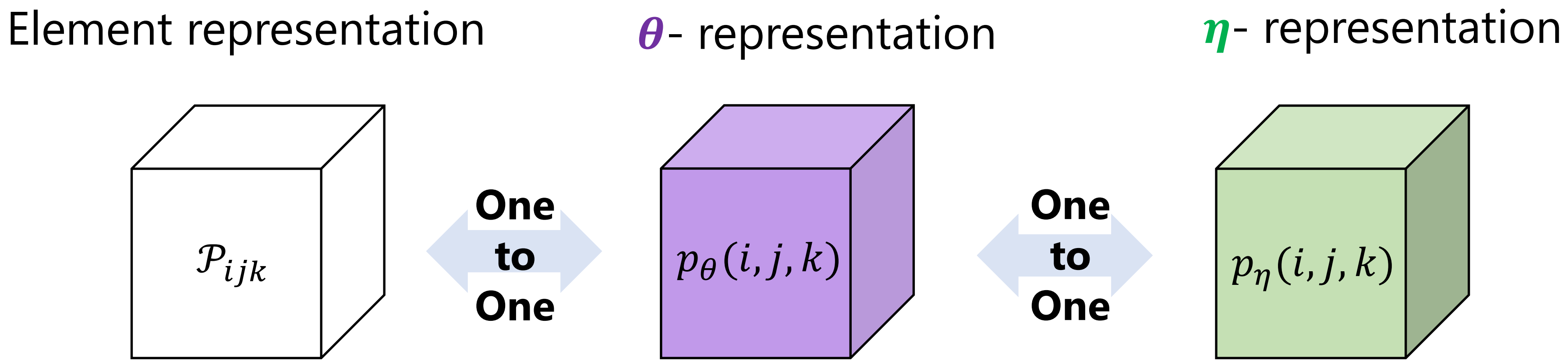
$$p_\eta(1,1,2) = \eta_{222} - \eta_{221} - \eta_{122} + \eta_{112}$$

$$p_\theta(i,j,k) = \exp\left[\sum_{i' \le i} \sum_{j' \le j} \sum_{k' \le k} \theta_{i'j'k'}\right]$$

**Relation between distribution and matrix**

Random Variable : index $i, j, k$
Sample space : index set
Value of the probability : element $P_{ijk}$

# Various representations of a normalized tensor




We can describe matrix properties by using $\boldsymbol{\theta}$- and $\boldsymbol{\eta}$- representations.

**Easier to formulate as a convex problem**.

# Describe the rank-1 condition of a tensor using $(\theta,\eta)$

**one-body parameters**

$\theta_{i11}, \theta_{1j1}, \theta_{11k} \qquad \eta_{i11}, \eta_{1j1}, \eta_{11k}$

Only one index is 1.

**many-body parameters**

A parameter other than a one-body parameter

**Rank-1 condition ($\boldsymbol{\theta}$-representation)**

$\mathrm{rank}(\mathcal{P}) = 1 \Leftrightarrow$ its all many − body $\theta$ parameters are 0

$(\Leftarrow)$

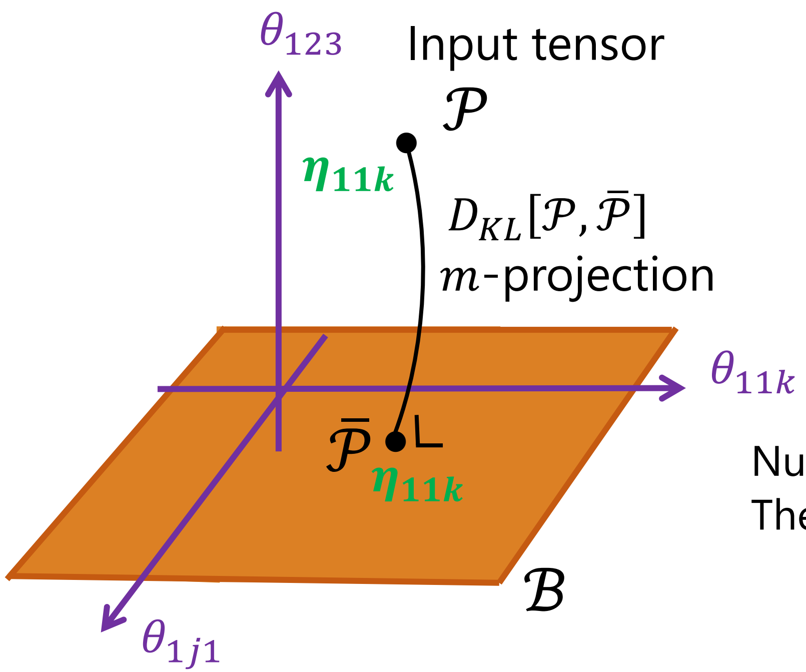
$$\mathcal{P}_{ijk} = \exp\left[\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}\theta_{ijk}\right] = \exp[\theta_{111}]\exp\left[\sum_{i=2}^{I}\theta_{i11}\right]\exp\left[\sum_{j=2}^{J}\theta_{1j1}\right]\exp\left[\sum_{k=2}^{K}\theta_{11k}\right]$$

$$\mathcal{P} = e^{\theta_{111}}\begin{pmatrix} 1 \\ e^{\theta_{211}} \\ e^{\theta_{211}+\theta_{311}} \\ \vdots \\ e^{\theta_{211}+\theta_{311}+\cdots+\theta_{I11}} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{\theta_{121}} \\ e^{\theta_{121}+\theta_{131}} \\ \vdots \\ e^{\theta_{121}+\theta_{131}+\cdots+\theta_{1J1}} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{\theta_{211}} \\ e^{\theta_{211}+\theta_{311}} \\ \vdots \\ e^{\theta_{211}+\theta_{311}+\cdots+\theta_{11K}} \end{pmatrix}$$

The rank of the tensor that can be represented by the Kronecker product of three vectors is 1 ∎

# Projection onto rank-1 space

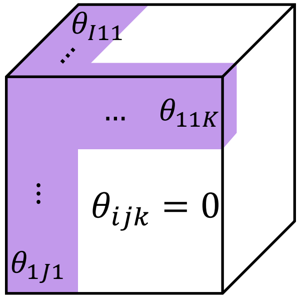
**The rank-1 approximation is a projection onto a subspace $\boldsymbol{\mathcal{B}}$ with all zero many-body natural parameters.**




The projection from any input tensor $\mathcal{P} \in \mathbb{R}_{>0}^{I\times J\times K}$ to $\mathcal{B}$ is convex.

But!! It takes too much time to get $\bar{\mathcal{P}}$ using the gradient method.😥😥

Projection from $\mathcal{P}$ *onto* $\mathcal{B}$




Number of natural parameters to optimize is $(I+J+K)$

The computational complexity of the Newton method is $O((I+J+K)^3)$

The one-body η is invariant to this $m$-projection

⟺ Summation in each axial direction is invariant for rank-1 approximation

➡ Let us describe the rank-1 condition with the expectation parameter $\boldsymbol{\eta}$.

# Describe the rank-1 condition using $(\theta,\eta)$

**Rank-1 condition ($\boldsymbol{\theta}$-representation)**

$\mathrm{rank}(\mathcal{P}) = 1 \Leftrightarrow$ its all many − body $\theta$ parameters are 0

⇕

**Rank-1 condition ($\boldsymbol{\eta}$-representation)**

$\mathrm{rank}(\mathcal{P}) = 1 \Leftrightarrow$ its all many − body $\eta$ parameters are factorizable as $\eta_{ijk} = \eta_{i11}\eta_{1j1}\eta_{11k}$

# The closed-formula of the best rank 1 approximation

Rank-1 condition ($\boldsymbol{\theta}$-representation)

$\mathrm{rank}(\mathcal{P}) = 1 \Leftrightarrow$ its all many − body $\theta$ parameters are 0

Rank-1 condition ($\boldsymbol{\eta}$-representation)

$\mathrm{rank}(\mathcal{P}) = 1 \Leftrightarrow$ its all many-body $\eta$ parameters are factorizable as $\eta_{ijk} = \eta_{i11}\eta_{1j1}\eta_{11k}$

**We derive a solution formula of the best rank-1 approximation.**

By the way, Frobenius error minimization is **NP-hard**

**Best rank-1 tensor formula for minimizing KL divergence** ($d = 3$ **)**

For any given positive tensor $\mathcal{P} \in \mathbb{R}_{>0}^{I\times J\times K}$, its best rank-1 approximation is

$$\bar{\mathcal{P}}_{ijk} = \left(\sum_{j'=1}^{J}\sum_{k'=1}^{K}\mathcal{P}_{ij'k'}\right)\left(\sum_{k'=1}^{K}\sum_{i'=1}^{I}\mathcal{P}_{i'jk'}\right)\left(\sum_{i'=1}^{I}\sum_{j'=1}^{J}\mathcal{P}_{i'j'k}\right),$$

that is, it is hold that

$$\bar{\mathcal{P}} = \underset{\mathcal{Q}:\mathrm{rank}(\mathcal{Q})=1}{\operatorname{argmin}} \; D_{\mathrm{KL}}(\mathcal{P};\mathcal{Q}).$$

We reproduce the result in K.Huang, et al. "Kullback-Leibler principal component for tensors is not NP-hard." *ACSSC* 2017

# Mean-field approximation and rank-1 approximation

**Best rank-1 tensor formula for minimizing KL divergence ($d = 3$)**

For any given positive tensor $\mathcal{P} \in \mathbb{R}_{>0}^{I \times J \times K}$, its best rank-1 approximation is

$$\bar{\mathcal{P}}_{ijk} = \left(\sum_{j'=1}^{J}\sum_{k'=1}^{K}\mathcal{P}_{ij'k'}\right)\left(\sum_{k'=1}^{K}\sum_{i'=1}^{I}\mathcal{P}_{i'jk'}\right)\left(\sum_{i'=1}^{I}\sum_{j'=1}^{J}\mathcal{P}_{i'j'k}\right)$$

Normalized vector depending on only $i$

Normalized vector depending on only $j$

Normalized vector depending on only $k$

A tensor with $d$ indices is a joint distribution with $d$ random variables.
A vector with only 1 index is an independent distribution with only one random variable.

**Rank-1 approximation approximates a joint distribution by a product of independent distributions.**

Mean-field approximation **: a methodology in physics for reducing a many-body problem to a one-body problem.**

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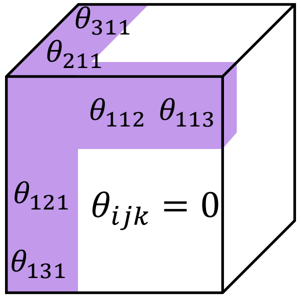
- Experiment
- Conclusion

# Formulate Tucker rank reduction by relaxing the rank-1 condition

**Rank-1 condition ($\boldsymbol{\theta}$-representation)**

$\mathrm{rank}(\mathcal{P}) = 1 \Leftrightarrow$ its all many-body $\theta$ parameters are 0




Expand the tensor by focusing on the $k$-th axis into a rectangular matrix $\theta^{(k)}$ (mode-$k$ expansion)

The first row and first column are the scaling factors

$$\theta^{(1)} = \begin{bmatrix} \theta_{111} & \theta_{121} & \theta_{131} & \theta_{112} & 0 & 0 & \theta_{113} & 0 & 0 \\ \theta_{211} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \theta_{311} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Two bingos

$$\theta^{(2)} = \begin{bmatrix} \theta_{111} & \theta_{211} & \theta_{311} & \theta_{112} & 0 & 0 & \theta_{311} & 0 & 0 \\ \theta_{121} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \theta_{131} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Two bingos

$$\theta^{(3)} = \begin{bmatrix} \theta_{111} & \theta_{211} & \theta_{311} & \theta_{121} & 0 & 0 & \theta_{131} & 0 & 0 \\ \theta_{112} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \theta_{113} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Two bingos

Rank (1,1,1)

# The relationship between bingo and rank

$$\theta^{(1)} = \begin{bmatrix} \theta_{111} & \theta_{121} & \theta_{131} & \theta_{112} & 0 & 0 & \theta_{113} & 0 & 0 \\ \theta_{211} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \theta_{311} & \theta_{321} & \theta_{331} & \theta_{312} & \theta_{322} & \theta_{332} & \theta_{313} & \theta_{323} & \theta_{333} \end{bmatrix}$$

→ One bingo

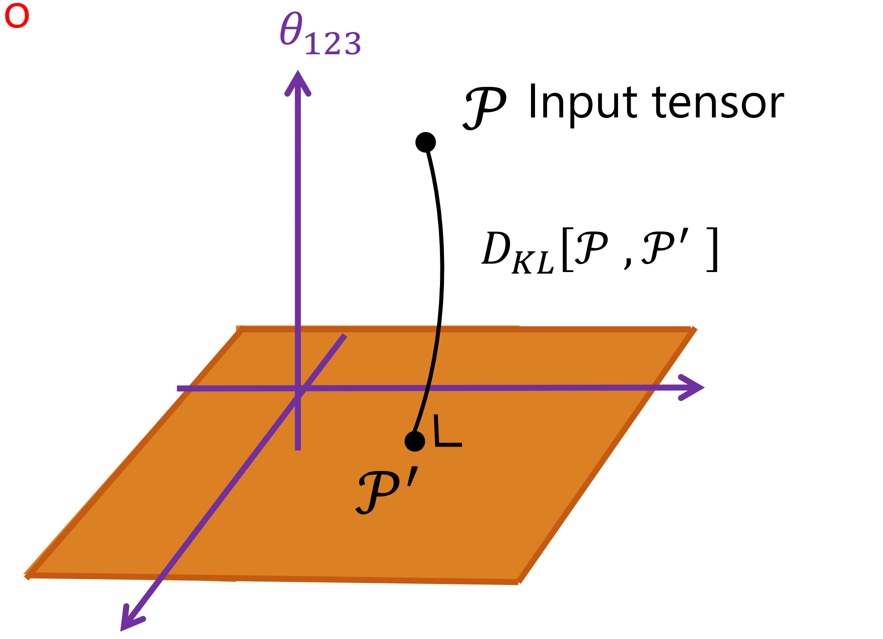
$$\theta^{(2)} = \begin{bmatrix} \theta_{111} & \theta_{211} & \theta_{311} & \theta_{112} & 0 & \theta_{312} & \theta_{311} & 0 & \theta_{313} \\ \theta_{121} & 0 & \theta_{321} & 0 & 0 & \theta_{322} & 0 & 0 & \theta_{323} \\ \theta_{131} & 0 & \theta_{331} & 0 & 0 & \theta_{332} & 0 & 0 & \theta_{333} \end{bmatrix}$$

No bingo

$$\theta^{(3)} = \begin{bmatrix} \theta_{111} & \theta_{211} & \theta_{311} & \theta_{121} & 0 & \theta_{321} & \theta_{131} & 0 & \theta_{331} \\ \theta_{112} & 0 & \theta_{312} & 0 & 0 & \theta_{322} & 0 & 0 & \theta_{332} \\ \theta_{113} & 0 & \theta_{313} & 0 & 0 & \theta_{323} & 0 & 0 & \theta_{333} \end{bmatrix}$$

No bingo

Rank (2,3,3)

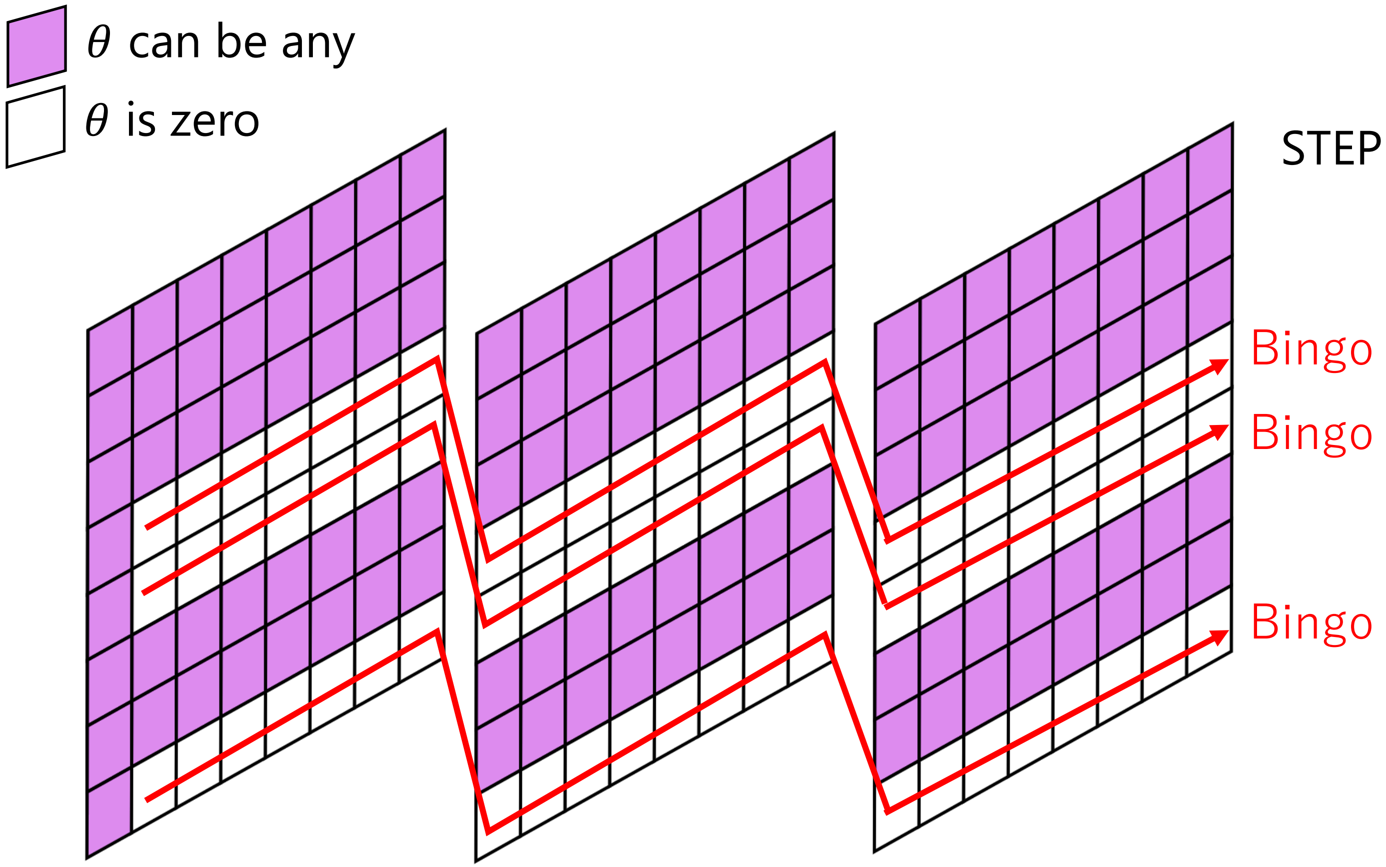



Subspace with one bingo in the mode-1 direction $\mathcal{B}^{(1)}$

**Bingo rule ($d = 3$)**

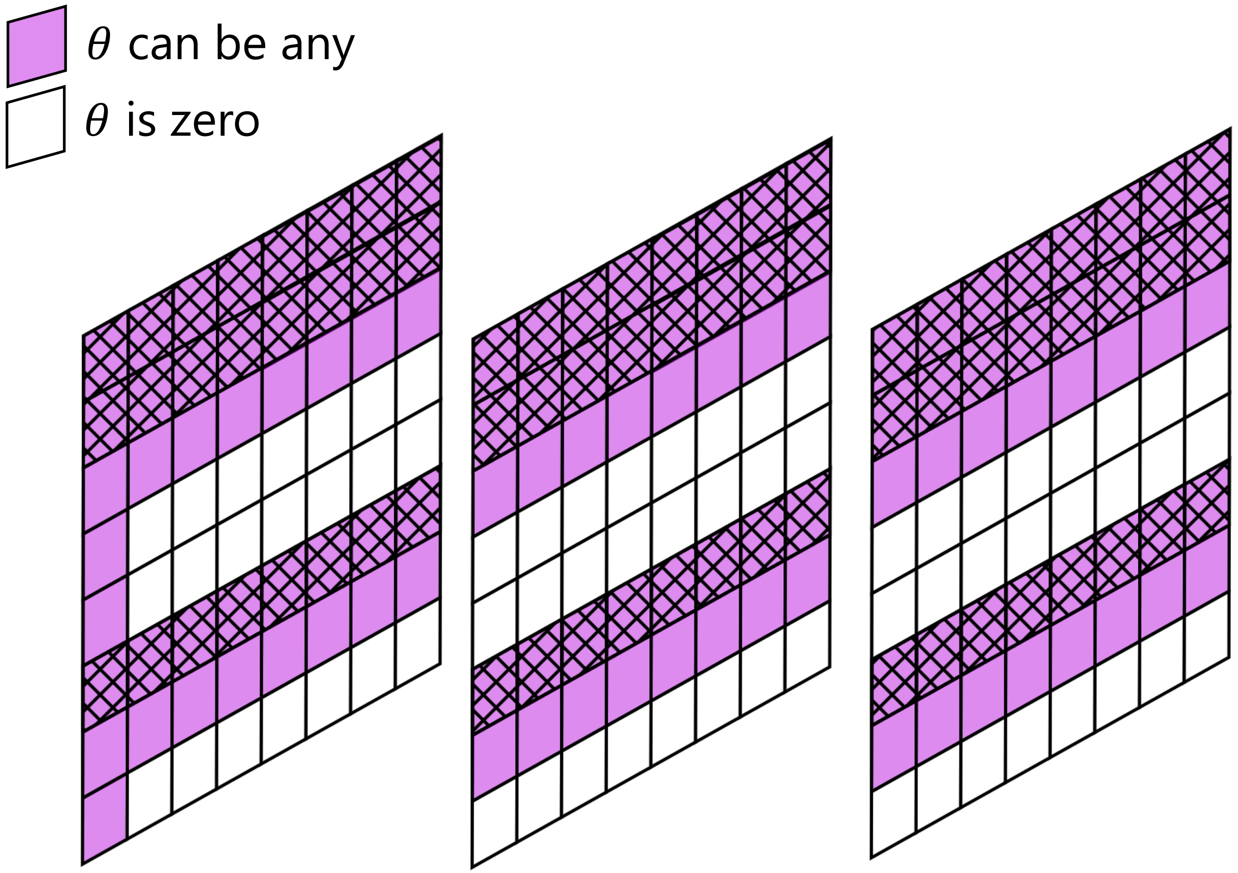
The mode-$k$ expansion $\theta^{(k)}$ of the natural parameter of a tensor $\mathcal{P} \in \mathbb{R}_{>0}^{I_1 \times I_2 \times I_3}$ has $b_k$ bingos
$\Rightarrow \mathrm{rank}(\mathcal{P}) \leq (I_1 - b_1, I_2 - b_2, I_3 - b_3)$

# Example: Reduce the rank of (8,8,3) tensor to (**5**,8,3) or less




STEP1 : Choose a bingo location.

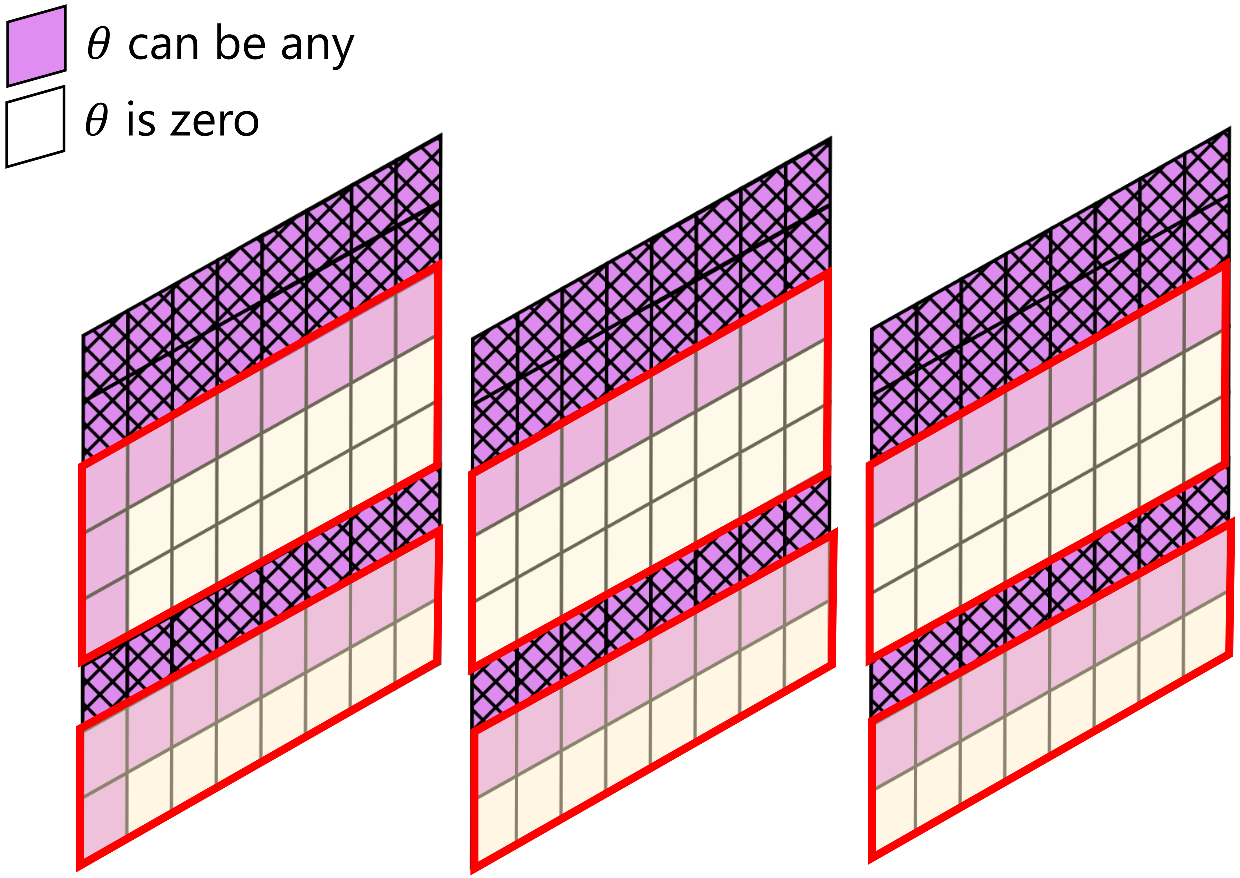
# Example: Reduce the rank of (8,8,3) tensor to (**5**,8,3) or less




STEP1 : Choose a bingo location.

The shaded areas do not change their values in the projection.

# Example: Reduce the rank of (8,8,3) tensor to (**5**,8,3) or less



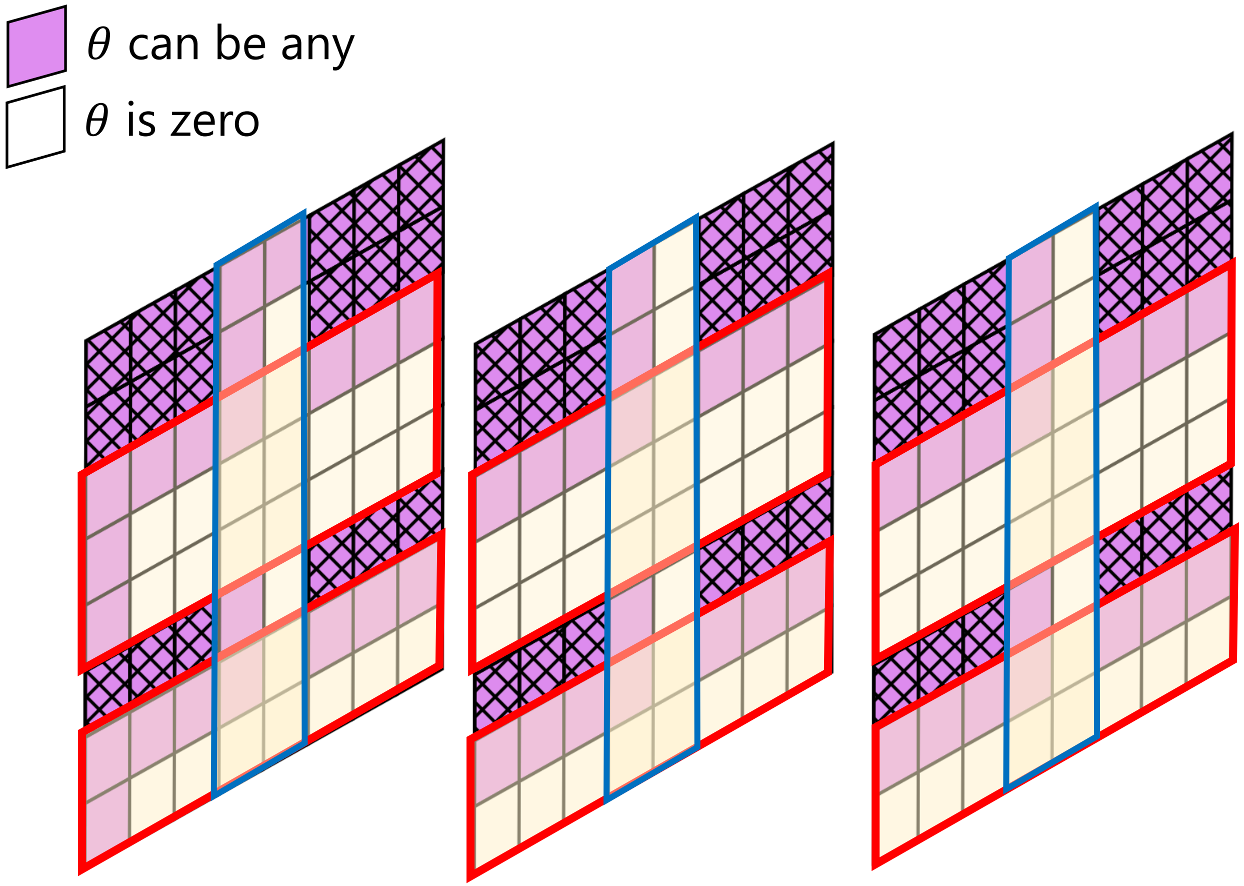

STEP1 : Choose a bingo location.

STEP2 : Replace the bingo part with the best rank-1 tensor.

Replace the partial tensor in the red box using the best rank 1 approximation formula

The best tensor is obtained in the specified bingo space. 😁
There is no guarantee that it is the best rank (5,8,3) approximation. 😥

# Example: Reduce the rank of (8,8,3) tensor to (**5**,**7**,3) or less.

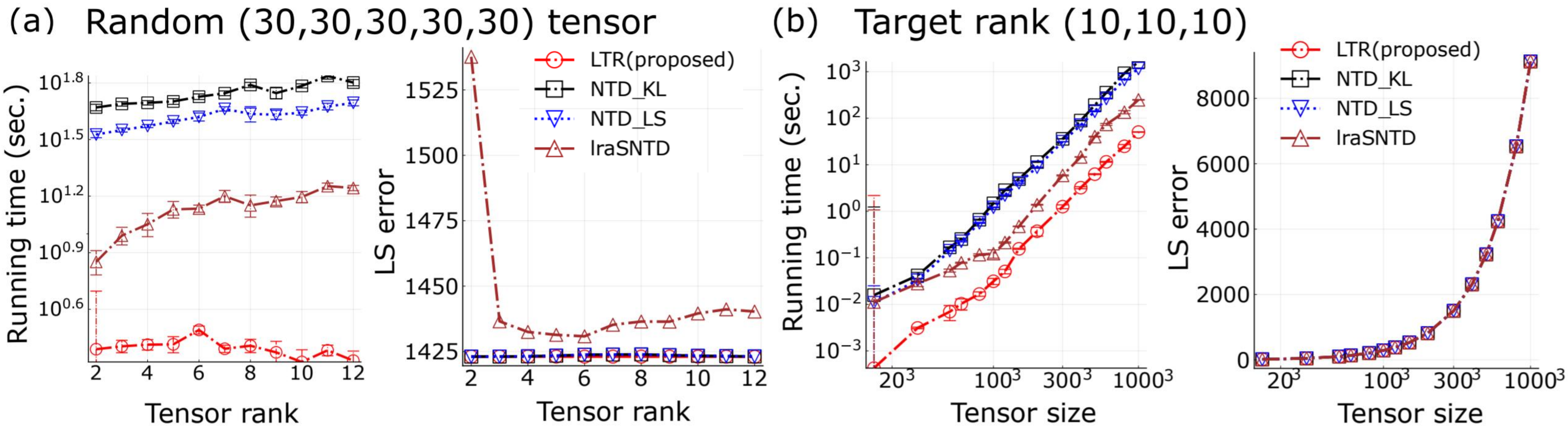



STEP1 : Choose a bingo location.

STEP2 : Replace the bingo part with the best rank-1 tensor.

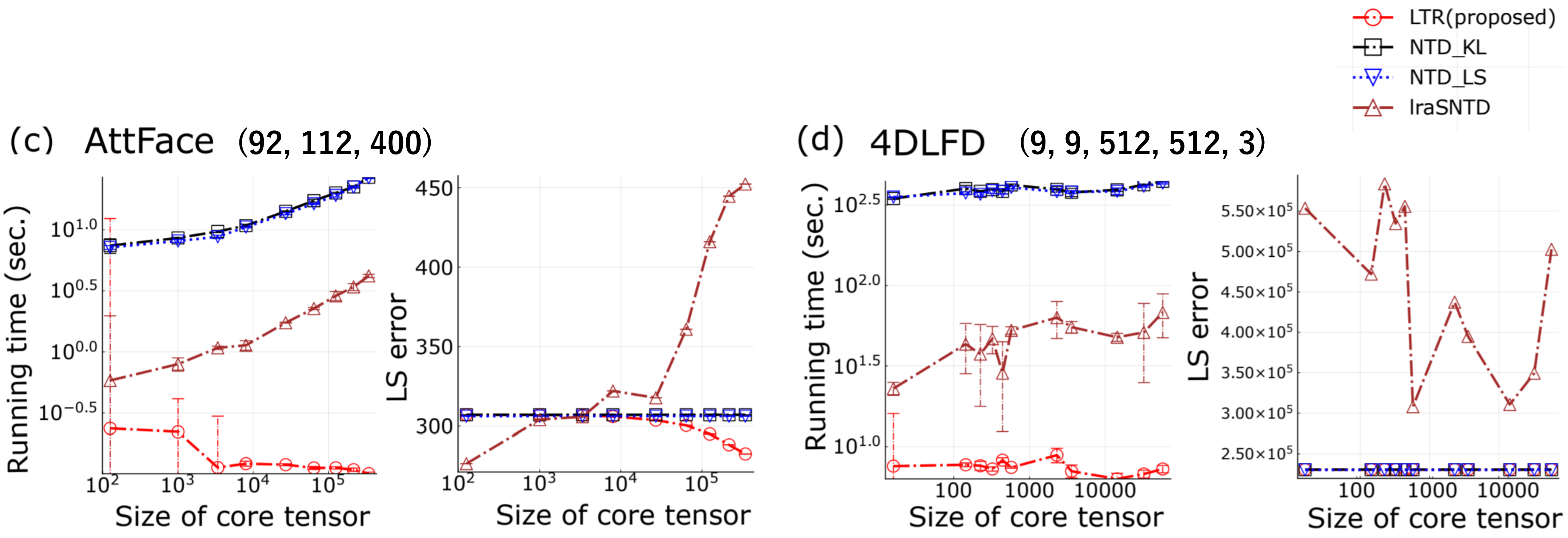
The shaded areas do not change in the projection.

# Experimental results (synthetic data)




**LTR is faster with the competitive approximation performance.**

# Experimental results (real data)




**LTR is faster with the competitive approximation performance.**

# Conclusion

■ Describe the rank-1 condition using $(\theta,\eta)$

Rank-1 condition ($\eta$-representation)

$$\bar{\eta}_{ijk} = \bar{\eta}_{i11}\bar{\eta}_{1j1}\bar{\eta}_{11k}$$

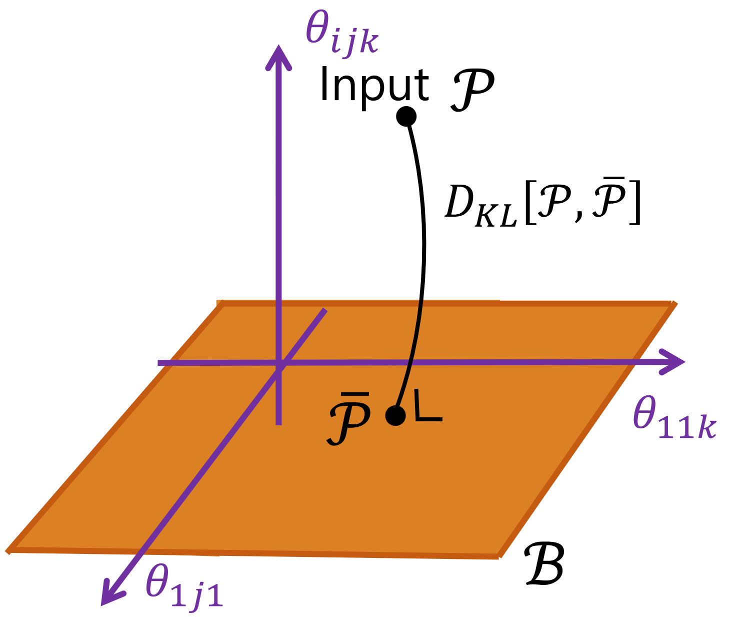
Low-rank condition ($\theta$-representation)

Bingo reduces rank

Rank-1 condition ($\theta$-representation)

All many body $\bar{\theta}_{ijk}$ are 0

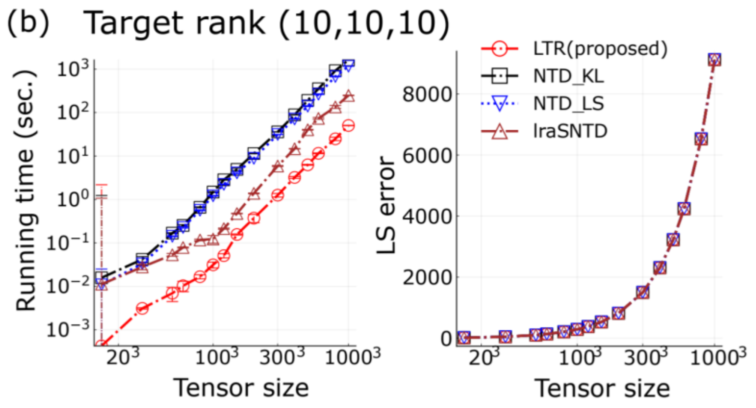
We discuss low-rank approximation as a problem of projection in $(\theta,\eta)$-space




■ Best rank-1 tensor formula for minimizing KL divergence

$$\bar{\mathcal{P}}_{ijk} = \left(\sum_{j'=1}^{J}\sum_{k'=1}^{K}\mathcal{P}_{ij'k'}\right)\left(\sum_{k'=1}^{K}\sum_{i'=1}^{I}\mathcal{P}_{ij'k'}\right)\left(\sum_{i'=1}^{I}\sum_{j'=1}^{J}\mathcal{P}_{i'j'k}\right)$$

■ Legendre Tucker Rank Reduction (LTR)




- LTR is based on mean-field approximation.
- LTR is faster with the competitive approximation performance as existing methods.
- No need to discuss learning rate, stopping criteria, or initial values