



Programs for
Junior Scientists



Many-body Approximation for Non-negative Tensors

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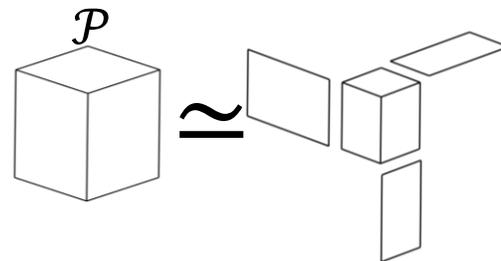
Difficulties in tensor factorization

Model selection is not intuitive.

CP decomp.

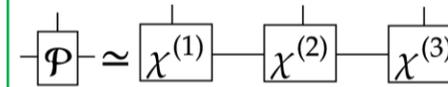


Tucker decomp.

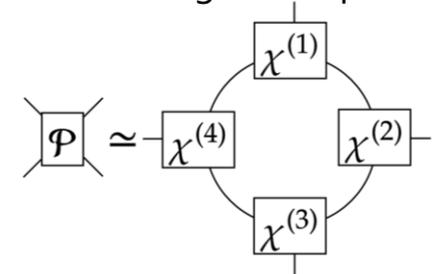


Decomp. with tensor networks

Tensor Train decomposition



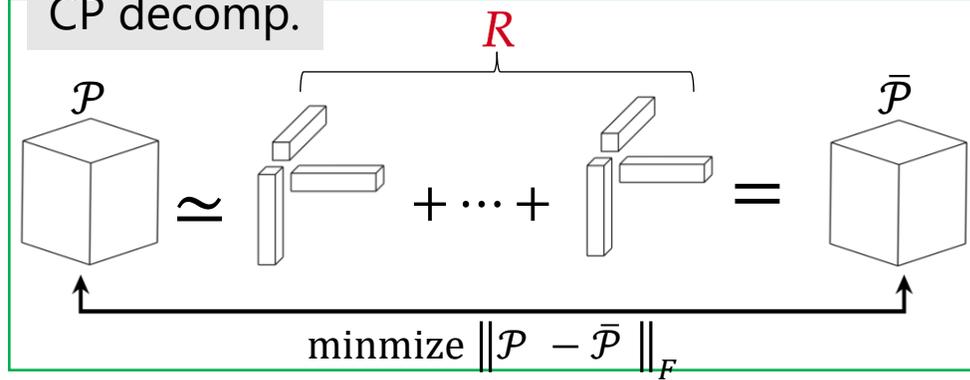
Tensor ring decomposition



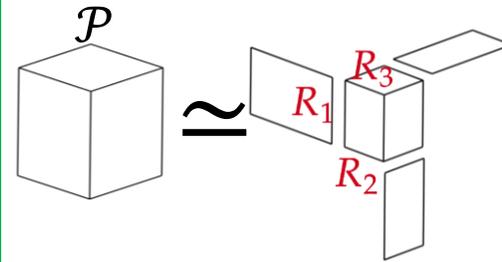
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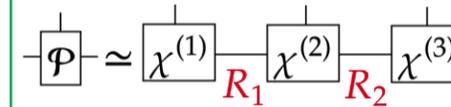


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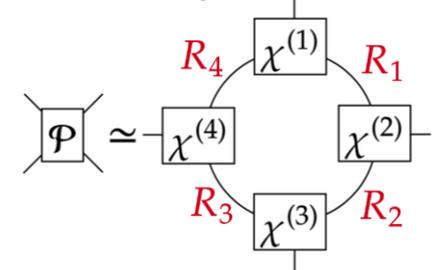


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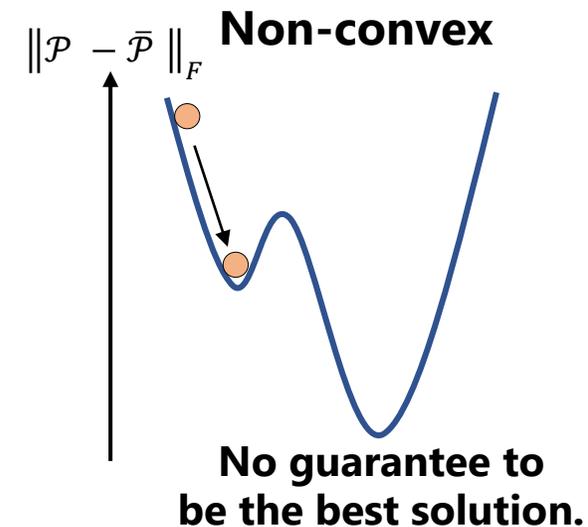


Optimization is difficult.

☹️ The objective function is typically **non-convex**.

- Initial values dependency

☹️ Solution often might be indeterminate.



A convex, stable and intuitive tensor factorization is desired.

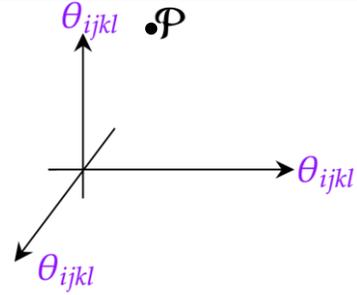
Many-body approximation for non-negative tensors

Energy function

$$\mathcal{P}_{ijkl} = \frac{1}{Z} \exp[-E_{\theta}(i, j, k, l)]$$

Natural parameter
of exponential distribution family.

$$\sum_{ijkl} \mathcal{P}_{ijkl} = 1$$



Many-body approximation for non-negative tensors

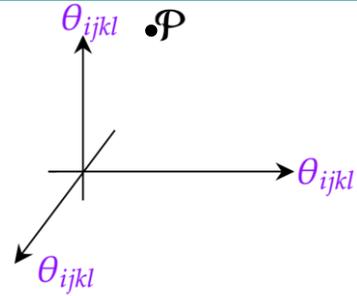
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$$= \frac{1}{Z} \exp \left[E_i^{(1)} + \dots + E_l^{(4)} + E_{ij}^{(12)} + \dots + E_{kl}^{(34)} + E_{ijk}^{(123)} + \dots + E_{jkl}^{(234)} + E_{ijkl}^{(1234)} \right]$$



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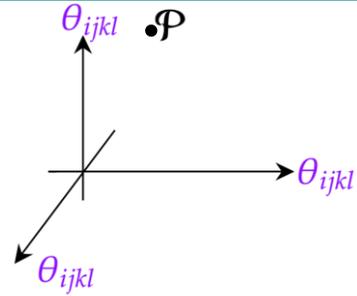
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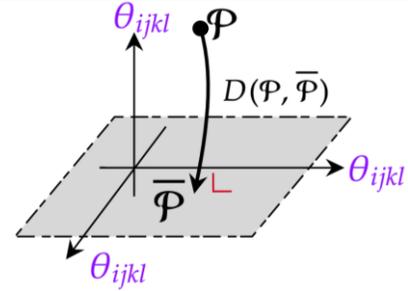
Control relation between
mode- k and mode- l .

Control relation among
mode- j , - k and - l .



Many-body approximation for non-negative tensors

$$\begin{aligned}\mathcal{P}_{ijkl} &= \frac{1}{Z} \exp[-E_{\theta}(i, j, k, l)] \\ &= \frac{1}{Z} \exp\left[E_i^{(1)} + \dots + E_l^{(4)} + E_{ij}^{(12)} + \dots + E_{kl}^{(34)} + E_{ijk}^{(123)} + \dots + E_{jkl}^{(234)} + E_{ijkl}^{(1234)} \right]\end{aligned}$$



One-body approx.

$$\bar{\mathcal{P}}_{ijkl} = p_i^{(1)} p_j^{(2)} p_k^{(3)} p_l^{(4)}$$

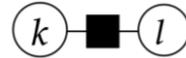
Rank-1 approximation (mean-field approximation)

[NeurIPS 2021 [Ghalamkari, K., Sugiyama, M.](#)]

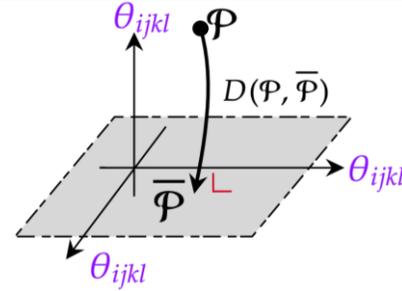
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Control relation between mode- k and mode- l .



One-body approx.

$$\bar{\mathcal{P}}_{ijkl} = p_i^{(1)} p_j^{(2)} p_k^{(3)} p_l^{(4)}$$

Two-body approx.

$$\bar{\mathcal{P}}_{ijkl} = X_{ij}^{(12)} X_{ik}^{(13)} X_{il}^{(14)} X_{jk}^{(23)} X_{jl}^{(24)} X_{kl}^{(34)}$$

**Rank-1 approximation
(mean-field approximation)**

[NeurIPS 2021 Ghalamkari, K., Sugiyama, M.]

Larger
Capability

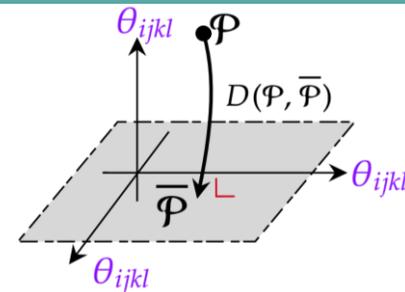
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One-body approx.

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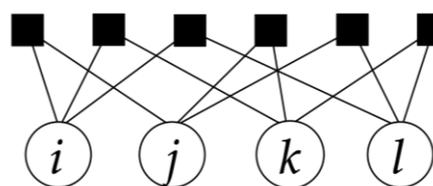


Rank-1 approximation
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Two-body approx.

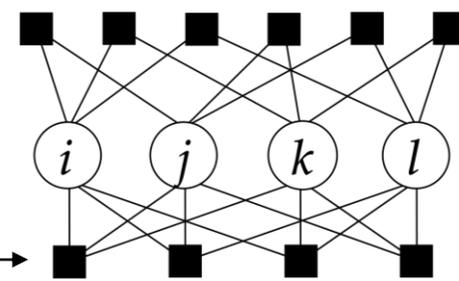
$$\bar{\mathcal{P}}_{ijkl} = X_{ij}^{(12)} X_{ik}^{(13)} X_{il}^{(14)} X_{jk}^{(23)} X_{jl}^{(24)} X_{kl}^{(34)}$$



Two-body Interaction

Three-body approx.

$$\bar{\mathcal{P}}_{ijkl} = \chi_{ijk}^{(123)} \chi_{ijl}^{(124)} \chi_{ikl}^{(134)} \chi_{jkl}^{(234)}$$



Three-body Interaction

Intuitive modeling focusing on interactions between modes

Larger Capability

The global optimal solution $\bar{\mathcal{P}}$ minimizing KL divergence from \mathcal{P} can be obtained by a convex optimization.

Theoretical idea behind proposal

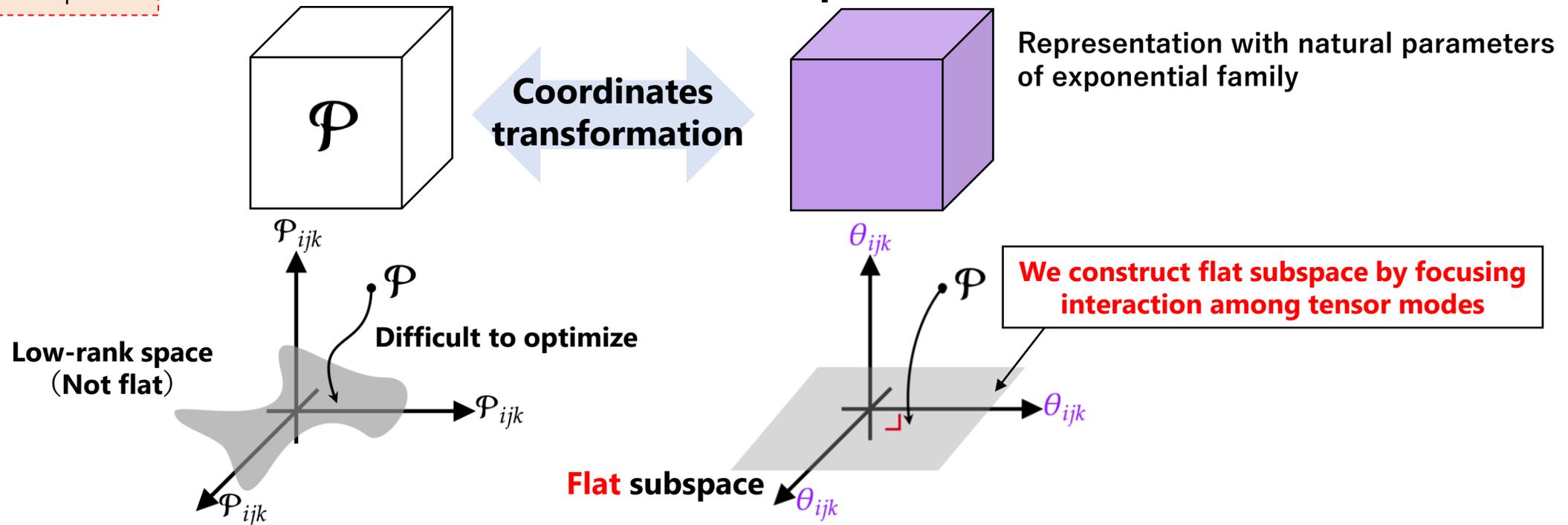
Index is discrete random variable

$$\sum_{ijk} \mathcal{P}_{ijk} = 1, \quad (i, j, k) \in \Omega = \{(1, 1, 1), \dots, (L, J, K)\}$$

- 💡 We regard a normalized tensor \mathcal{P} as a discrete joint probability distribution whose sample space is an index set
- 💡 We use information geometry to formulate factorization as convex problem

Geometry of θ -space

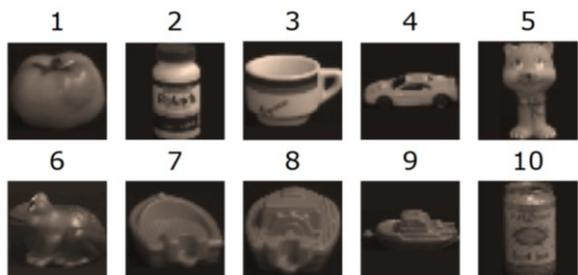
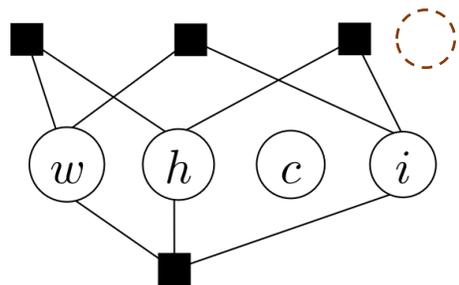
θ -Representation



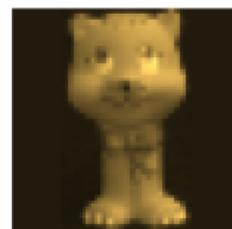
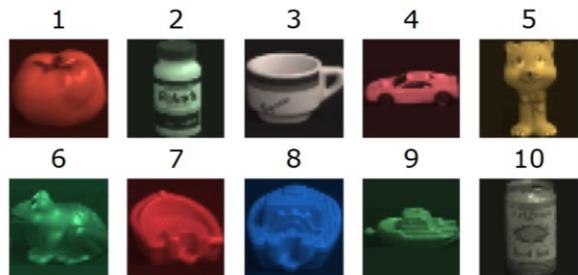
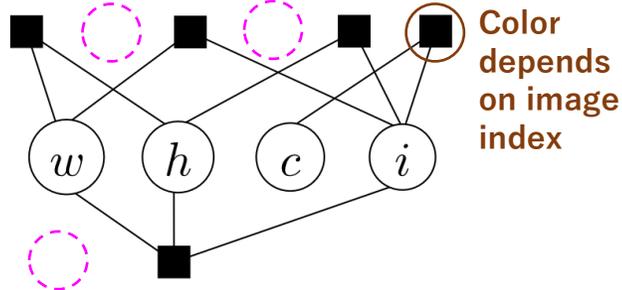
Describing tensor factorization in θ -coordinate system makes it convex problem

Reconstruction for $40 \times 40 \times 3 \times 10$ tensor

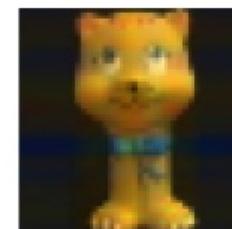
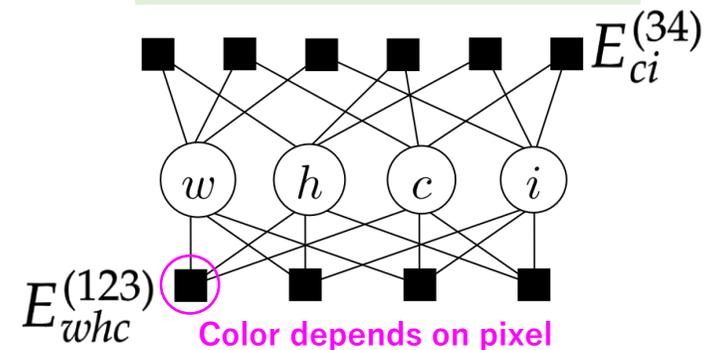
(Width, height, Colors, # images)



Color is uniform within each image.



Three-body Approx.



Larger
Quality

Intuitive model design that captures the relationship between modes

Rank-free convex nonnegative tensor factorization

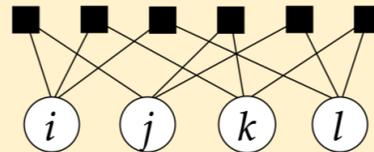
Many-body Approximation

$$\begin{aligned}\mathcal{P}_{ijkl} &= \exp \left[\sum_{i'=1}^i \sum_{j'=1}^j \sum_{k'=1}^k \sum_{l'=1}^l \theta_{i'j'k'l'} \right] \\ &= \frac{1}{Z} \exp \left[E_i^{(1)} + \dots + E_l^{(4)} + E_{ij}^{(12)} + \dots + E_{kl}^{(34)} + E_{ijk}^{(123)} + \dots + E_{jkl}^{(234)} + E_{ijkl}^{(1234)} \right]\end{aligned}$$

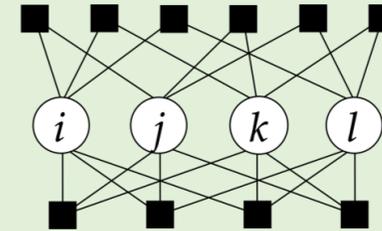
One-body Approx.



Two-body Approx.



Three-body Approx.



- Convex optimization always provide unique solution
- More intuitive design than rank tuning