

Probabilistic PCA on Tensors

(arXiv:2510.19516)

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OCAMI Workshop 2025

Tensor Basics

Basic terminology

Matrix: $M = [M_{i_1 i_2}] \in \mathbb{R}^{n_1 \times n_2}$.

Tensor: $T = [T_{i_1 i_2 \dots i_r}] \in \mathbb{R}^{n_1 \times n_2 \times \dots \times n_r}, \quad r = 1, 2, 3, \dots$

Basic terminology

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Tensor: $\mathbf{T} = [\mathbf{T}_{\mathbf{i}_1 \mathbf{i}_2 \cdots \mathbf{i}_r}] \in \mathbb{R}^{\mathbf{n}_1 \times \mathbf{n}_2 \times \cdots \times \mathbf{n}_r}, \quad r = 1, 2, 3, \dots$

Rank one matrix: $\mathbf{M} = \mathbf{u}_1 \mathbf{u}_2^\top, \quad \mathbf{u}_1 \in \mathbb{R}^{\mathbf{n}_1}, \mathbf{u}_2 \in \mathbb{R}^{\mathbf{n}_2}$.

$$\mathbf{M}_{\mathbf{i}_1 \mathbf{i}_2} = (\mathbf{u}_1)_{\mathbf{i}_1} (\mathbf{u}_2)_{\mathbf{i}_2}$$

Rank one tensor: $\mathbf{T} = \mathbf{u}_1 \otimes \cdots \otimes \mathbf{u}_r, \quad \mathbf{u}_i \in \mathbb{R}^{\mathbf{n}_i} \text{ for } i = 1, \dots, r$

$$\mathbf{T}_{\mathbf{i}_1 \cdots \mathbf{i}_r} = (\mathbf{u}_1)_{\mathbf{i}_1} \cdots (\mathbf{u}_r)_{\mathbf{i}_r}$$

Multilinear action on tensors

Matrix $\mathbf{A} \in \mathbb{R}^{n_1 \times m_1}$ acts on $\mathbf{v} \in \mathbb{R}^{m_1}$: $\mathbf{v} \mapsto \mathbf{Av} \in \mathbb{R}^{n_1}$.

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Matrices $\mathbf{A} \in \mathbb{R}^{n_1 \times m_1}$, $\mathbf{B} \in \mathbb{R}^{n_2 \times m_2}$ act on $\mathbf{M} \in \mathbb{R}^{m_1 \times m_2}$

$$\mathbf{M} \mapsto (\mathbf{A}, \mathbf{B}) \cdot \mathbf{M} := \mathbf{AMB}^\top \in \mathbb{R}^{n_1 \times n_2}$$

Note: $[\mathbf{AMB}^\top]_{i_1 i_2} = \sum_{j_1 j_2} \mathbf{A}_{i_1 j_1} \mathbf{B}_{i_2 j_2} \mathbf{M}_{j_1 j_2}$.

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Matrices $\mathbf{A}_1 \in \mathbb{R}^{n_1 \times m_1}, \dots, \mathbf{A}_r \in \mathbb{R}^{n_r \times m_r}$ act on $\mathbf{T} \in \mathbb{R}^{m_1 \times \dots \times m_r}$

$$\mathbf{T} \mapsto (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{T} \in \mathbb{R}^{n_1 \times \dots \times n_r}$$

where $[(\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{T}]_{i_1 \dots i_r} = \sum_{j_1, \dots, j_r} (\mathbf{A}_1)_{i_1 j_1} \cdots (\mathbf{A}_r)_{i_r j_r} \mathbf{T}_{j_1 \cdots j_r}$.

Tucker decomposition

Singular Value Decomposition: For every matrix $\mathbf{M} \in \mathbb{R}^{n_1 \times n_2}$ s.t. $\text{rank}(\mathbf{M}) \leq s$ there exist $\mathbf{U} \in \mathbb{R}^{n_1 \times s}$ and $\mathbf{V} \in \mathbb{R}^{n_2 \times s}$ such that and

$$\mathbf{M} = \mathbf{U}\mathbf{D}\mathbf{V}^\top = (\mathbf{U}, \mathbf{V}) \cdot \mathbf{D}$$

with $\mathbf{U}^\top \mathbf{U} = \mathbf{V}^\top \mathbf{V} = \mathbb{I}_s$ and $\mathbf{D} = \text{diag}(\sigma_1, \dots, \sigma_s) \in \mathbb{R}^{s \times s}$.

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A similar statement is true for only very special tensors. Nevertheless...

Tucker decomposition: For $\mathbf{T} \in \mathbb{R}^{n_1 \times \dots \times n_r}$ and $m_1 \leq n_1, \dots, m_r \leq n_r$ approximate:

$$\mathbf{T} \approx (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{S},$$

where $\mathbf{S} \in \mathbb{R}^{m_1 \times \dots \times m_r}$ is called the core tensor ("multivariate SVD").

Tensor PPCA

PPCA: Probabilistic Principle Component Analysis

PPCA (Tipping & Bishop, 1999): For a random vector $\mathbf{X} \in \mathbb{R}^n$:

$$\mathbf{X} = \mu + \mathbf{A}\mathbf{Z} + \mathbf{\epsilon}, \quad \mu \in \mathbb{R}^n, \mathbf{A} \in \mathbb{R}^{n \times m}, m \leq n,$$

$$\mathbf{Z} \sim \mathcal{N}_m(\mathbf{0}, \mathbb{I}_m), \quad \mathbf{\epsilon} \sim \mathcal{N}_n(\mathbf{0}, \sigma^2 \mathbb{I}_n), \quad \mathbf{Z} \perp \mathbf{\epsilon}.$$

Geometry: samples concentrate around the $\mu + \text{Im}(\mathbf{A})$; $\text{rank}(\mathbf{A}) = m$.

Note: We can assume $\mathbf{A}^\top \mathbf{A}$ is diagonal (column orthogonal).

- $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$, $\mathbf{V} \in \mathbb{R}^{m \times m}$ orthogonal, and $\mathbf{V}^\top \mathbf{Z} \stackrel{d}{=} \mathbf{Z}$; thus $\mathbf{V} = \mathbb{I}_m$ w.l.o.g.

Tensor PPCA

Suppose now $\mathbf{X} \in \mathbb{V} := \mathbb{R}^{n_1 \times \dots \times n_r}$ is a tensor.

Tensor PCA model: \mathbf{X} admits stochastic representation

$$\mathbf{X} = \mu + (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{Z} + \mathbf{E},$$

where $\mathbf{Z} \in \mathbb{U} := \mathbb{R}^{m_1 \times \dots \times m_r}$ standard normal, $\mathbf{E} \in \mathbb{V}$ isotropic, $\mathbf{Z} \perp\!\!\!\perp \mathbf{E}$.

Dimension reduction assuming: $\mu = \mathbf{0}$ or $\mu = (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \boldsymbol{\nu}$.

Natural questions: identifiability, estimation, learning $\mathbf{m}_1, \dots, \mathbf{m}_r$.

The distribution of \mathbf{X} is Gaussian

Recall: $\mathbf{X} = (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{Z} + \mathbf{E}$ (we assumed zero mean)

Inner product on \mathbb{V} : $\langle \mathbf{S}, \mathbf{T} \rangle := \sum_{i_1, \dots, i_r} \mathbf{S}_{i_1 \dots i_r} \mathbf{T}_{i_1 \dots i_r}, \quad \|\mathbf{T}\|_F = \sqrt{\langle \mathbf{T}, \mathbf{T} \rangle}.$

$$\langle \mathbf{X}, \mathbf{T} \rangle = \langle (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{Z}, \mathbf{T} \rangle + \langle \mathbf{E}, \mathbf{T} \rangle = \langle \mathbf{Z}, (\mathbf{A}_1^\top, \dots, \mathbf{A}_r^\top) \cdot \mathbf{T} \rangle + \langle \mathbf{E}, \mathbf{T} \rangle$$

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We conclude: $\langle \mathbf{X}, \mathbf{T} \rangle \sim \mathbf{N}(\mathbf{0}, \|(\mathbf{A}_1^\top, \dots, \mathbf{A}_r^\top) \cdot \mathbf{T}\|_F^2 + \|\mathbf{T}\|_F^2).$

The distribution of \mathbf{X} is Gaussian

Recall: $\mathbf{X} = (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{Z} + \mathbf{E}$ (we assumed zero mean)

Inner product on \mathbb{V} : $\langle \mathbf{S}, \mathbf{T} \rangle := \sum_{i_1, \dots, i_r} \mathbf{S}_{i_1 \dots i_r} \mathbf{T}_{i_1 \dots i_r}$, $\|\mathbf{T}\|_F = \sqrt{\langle \mathbf{T}, \mathbf{T} \rangle}$.

$$\langle \mathbf{X}, \mathbf{T} \rangle = \langle (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{Z}, \mathbf{T} \rangle + \langle \mathbf{E}, \mathbf{T} \rangle = \langle \mathbf{Z}, (\mathbf{A}_1^\top, \dots, \mathbf{A}_r^\top) \cdot \mathbf{T} \rangle + \langle \mathbf{E}, \mathbf{T} \rangle$$

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Covariance operator: $\Sigma : \mathbb{V} \rightarrow \mathbb{V}$ is the linear function

$$\Sigma(\mathbf{T}) = \sigma^2 \mathbf{T} + (\mathbf{A}_1 \mathbf{A}_1^\top, \dots, \mathbf{A}_r \mathbf{A}_r^\top) \cdot \mathbf{T}$$

Now $\langle \mathbf{X}, \mathbf{T} \rangle \sim \mathbf{N}(\mathbf{0}, \langle \Sigma(\mathbf{T}), \mathbf{T} \rangle)$. (generalizes multivariate normal)

First results

Spectrum of Σ

Recall: $\Sigma : \mathbb{V} \rightarrow \mathbb{V}$ satisfies $\Sigma(\mathbf{T}) = \sigma^2 \mathbf{T} + (\mathbf{A}_1 \mathbf{A}_1^\top, \dots, \mathbf{A}_r \mathbf{A}_r^\top) \cdot \mathbf{T}$

Let $\mathbf{u}_i^{(k)}, \lambda_i^{(k)}$ be the eigenvectors and eigenvalues of $\mathbf{B}_k = \mathbf{A}_k \mathbf{A}_k^\top$.

$$\Sigma(\mathbf{u}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{u}_{i_r}^{(r)}) = (\sigma^2 + \lambda_{i_1}^{(1)} \cdots \lambda_{i_r}^{(r)}) \cdot \mathbf{u}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{u}_{i_r}^{(r)}$$

- at most $\mathbf{m}_1 \cdots \mathbf{m}_r$ eigenvalues greater than σ^2 ($\text{rank}(\mathbf{B}_k) \leq \mathbf{m}_k$),
- remaining $\mathbf{n}_1 \cdots \mathbf{n}_r - \mathbf{m}_1 \cdots \mathbf{m}_r$ eigenvalues are all equal to σ^2 .

Σ has rich structure both in eigenvalues and eigenvectors!

Model identifiability

Recall: $\mathbf{X} = (\mathbf{A}_1, \dots, \mathbf{A}_r) \cdot \mathbf{Z} + \mathbf{E}$

Assumption 1: Each \mathbf{A}_k is column orthogonal.

Assumption 2: $\|\mathbf{B}_1\|_F = \dots = \|\mathbf{B}_r\|_F$, where $\mathbf{B}_k := \mathbf{A}_k \mathbf{A}_k^\top$.

Assumption 3: Either $n_k > m_k$ for at least one k or at least two of the \mathbf{B}_k are not scalar matrices.

Theorem: Under Assumptions 1-3 the parameters $\mathbf{A} = (\mathbf{A}_1, \dots, \mathbf{A}_r)$ and σ^2 are identifiable.

Existence of the MLE

Observation: The MLE for standard PPCA model exists (with probability one) if and only if the sample size N satisfies $N > m$.

Theorem: In TPCA suppose $n_k > m_k$ for some k . Then the MLE exists with probability 1 even for $N = 1$.

To find the MLE we perform the EM algorithm.

This is a computationally expensive procedure.

Next, we study a **computationally efficient estimator**.

Alternative estimator

Pair reshaping

Recall: $\Sigma : \mathbb{V} \rightarrow \mathbb{V}$, $\mathbb{V} = \mathbb{R}^{n_1 \times \cdots \times n_r}$; slightly abusing notation $\Sigma \in \mathbb{R}^{n_1 \times \cdots \times n_r \times n_1 \times \cdots \times n_r}$

The **pair-reshaping** operator $\text{PAIR}(\cdot)$ that maps Σ to $\mathbb{R}^{n_1^2 \times \cdots \times n_r^2}$:

$$\text{PAIR}(\Sigma) = \text{VEC}(\mathbf{B}_1) \otimes \cdots \otimes \text{VEC}(\mathbf{B}_r) + \sigma^2 \text{VEC}(\mathbb{I}_{n_1}) \otimes \cdots \otimes \text{VEC}(\mathbb{I}_{n_r}).$$

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In the Frobenius norm, the first term massively dominates.

So $\text{PAIR}(\Sigma)$ is **approximately rank one**. In addition:

$$\left\langle \frac{\mathbf{B}_k}{\|\mathbf{B}_k\|_F}, \frac{\mathbb{I}_{n_k}}{\|\mathbb{I}_{n_k}\|_F} \right\rangle = \frac{\text{tr}(\mathbf{B}_k)}{\|\mathbf{B}_k\|_F \sqrt{n_k}} \leq \sqrt{\frac{m_k}{n_k}}$$

Finding a rank one approximation to a given tensor is a very classical problem in tensors and is solved using the **power method**.

Power method for matrices

For a general matrix \mathbf{M} , the best rank-1 approximation $\mathbf{M} \approx \sigma_1 \mathbf{u}_1 \mathbf{v}_1^\top$ is obtained from its principal left/right singular vectors.

Alternating power iteration: $\mathbf{u}_{t+1} = \frac{\mathbf{M}\mathbf{v}_t}{\|\mathbf{M}\mathbf{v}_t\|}, \quad \mathbf{v}_{t+1} = \frac{\mathbf{M}^\top \mathbf{u}_{t+1}}{\|\mathbf{M}^\top \mathbf{u}_{t+1}\|}.$

In Tucker notation: $\mathbf{M}\mathbf{v} = (\mathbb{I}, \mathbf{v}) \cdot \mathbf{M}, \quad \mathbf{M}^\top \mathbf{u} = (\mathbf{u}, \mathbb{I}) \cdot \mathbf{M}.$

Our tensor algorithm uses exactly this idea: a rank-1 power method extended from 2 modes to r modes; e.g. $\mathbf{u}_1 \leftarrow (\mathbb{I}, \mathbf{u}_2, \dots, \mathbf{u}_r) \cdot \mathbf{T} / \|\cdot\|$.

Rank-1 power iteration

Recall: $\text{PAIR}(\boldsymbol{\Sigma}) = \text{VEC}(\mathbf{B}_1) \otimes \cdots \otimes \text{VEC}(\mathbf{B}_r) + \sigma^2 \text{VEC}(\mathbb{I}_{n_1}) \otimes \cdots \otimes \text{VEC}(\mathbb{I}_{n_r})$.

$$\text{PAIR}(\boldsymbol{\Sigma}) = \mathbf{b}_1 \otimes \cdots \otimes \mathbf{b}_r + \text{small perturbation}$$

By Assumption 2, the norms of $\mathbf{b}_1, \dots, \mathbf{b}_r$ are all equal; say $\omega^{1/r}$.

$$\text{PAIR}(\boldsymbol{\Sigma}) = \omega \mathbf{b}_1 \otimes \cdots \otimes \mathbf{b}_r + \text{small perturbation}, \quad \|\mathbf{b}_1\| = \cdots = \|\mathbf{b}_r\| = 1$$

Rank-1 power iteration

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Let $\text{PAIR}(\mathbf{S}_N)$ be a sample estimator of $\text{PAIR}(\boldsymbol{\Sigma})$. Our procedure finds:

$$\text{PAIR}(\mathbf{S}_N) \approx \hat{\omega} \hat{\mathbf{b}}_1 \otimes \cdots \otimes \hat{\mathbf{b}}_r$$

Additional regularization: Each $\hat{\mathbf{b}}_i$ is a vectorization of a low-rank matrix.

Probabilistic guarantees

The right norm

Recall, $\Sigma : \mathbb{V} \rightarrow \mathbb{V}$ given by $\Sigma(\mathbf{T}) = \sigma^2 \mathbf{T} + (\mathbf{A}_1 \mathbf{A}_1^\top, \dots, \mathbf{A}_r \mathbf{A}_r^\top) \cdot \mathbf{T}$.

“Standard” operator norm of $\mathbf{F} : \mathbb{V} \rightarrow \mathbb{V}$:

$$\|\mathbf{F}\|_{\text{op}} = \max_{\|\mathbf{T}\|_F=1} \|\mathbf{F}(\mathbf{T})\|_F = \max_{\|\mathbf{S}\|_F=\|\mathbf{T}\|_F=1} \langle \mathbf{F}(\mathbf{T}), \mathbf{S} \rangle.$$

We work with a weaker norm.

$$\mathbb{B} := \{\mathbf{u} = \mathbf{u}_1 \otimes \cdots \otimes \mathbf{u}_r : \|\mathbf{u}_1\| = \cdots = \|\mathbf{u}_r\| = 1\} \subseteq \mathbb{V}$$

$$\|\mathbf{F}\| := \max_{\mathbf{u}, \mathbf{v} \in \mathbb{B}} \langle \mathbf{F}(\mathbf{u}), \mathbf{v} \rangle.$$

Concentration

With \mathbf{N} samples, with high probability,

$$\|\mathbf{S}_{\mathbf{N}} - \boldsymbol{\Sigma}\| \lesssim \underbrace{\sigma^2 \phi_1\left(\frac{\sum n_k}{N}\right)}_{\text{noise}} + \underbrace{\|\mathbf{A}\|^2 \phi_2\left(\frac{\sum m_k}{N}\right)}_{\text{signal}} + \underbrace{\sigma \|\mathbf{A}\| \phi_3\left(\frac{\sum n_k + m_k}{N}\right)}_{\text{cross}}.$$

Here:

- ϕ_i are dimension-dependent rates specified in the paper.
- $\|\mathbf{A}\| := \|\mathbf{A}_1\| \cdots \|\mathbf{A}_r\|$

$$\frac{\|\mathbf{S}_{\mathbf{N}} - \boldsymbol{\Sigma}\|}{\|\mathbf{A}\|^2} \rightarrow 0 \text{ in probability as long as } \max\left\{\frac{n_{\max}}{\|\mathbf{A}\|^2}, \mathbf{m}_{\max}, \frac{n_{\max}}{\|\mathbf{A}\|}\right\} \frac{\log N}{N} \rightarrow 0.$$

One-step consistency

Recall: $\text{PAIR}(\mathbf{S}_N) \approx \omega \mathbf{b}_1 \otimes \cdots \otimes \mathbf{b}_r$, $\|\mathbf{b}_k\| = 1$. Use power iteration.

ψ = the RHS in the previous slide (small); $\omega = \prod_k \|\mathbf{B}_k\|_F$ (large).

$\theta_k^{(t)}$ = the angle between \mathbf{b}_k and $\mathbf{b}_k^{(t)}$ for $t = 0, 1, 2, \dots$

$c := \cos^2(\theta_k^{(0)}) \in (0, 1)$. (we need it to be bounded away from 0)

Theorem: Under mild assumptions: $\sin \theta_k^{(1)} \leq \frac{\psi}{\omega} \cdot \frac{\sqrt{m_1 \cdots m_r}}{c^{(r-1)/2}}$.

Moreover, $\left| \frac{\omega - \hat{\omega}^{(1)}}{\omega} \right| \leq \left(\frac{\psi}{\omega} \right)^2 \frac{16 r m_1 \cdots m_r}{c^{r-1}}$.

Discussion

Multilinear SVD give **deterministic** low-rank practical approximations.

But they lack:

- a probabilistic model for the noise or likelihood for inference,
- uncertainty quantification,
- principled model selection for the ranks \mathbf{m}_k .

Our contribution: a probabilistic multilinear model with identifiability, MLE existence, efficient estimation, and probabilistic guarantees.

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Our contribution: a probabilistic multilinear model with identifiability, MLE existence, efficient estimation, and probabilistic guarantees.

Thank you!

The paper, arXiv:2510.19516.

<https://pzwiernik.github.io/slides/tpca-ocami-2025.pdf>