

# Probabilistic PCA on Tensors

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Piotr Zwiernik



**Universitat  
Pompeu Fabra**  
*Barcelona*

Statistics, Probability  
and Machine Learning  
Research Group

joint work with Yaoming Zhen (CUHK, Shenzhen)

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# Tensor Basics

# Basic terminology

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

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

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Rank one matrix:  $\mathbf{M} = \mathbf{u}_1 \mathbf{u}_2^\top$ ,  $\mathbf{u}_1 \in \mathbb{R}^{n_1}$ ,  $\mathbf{u}_2 \in \mathbb{R}^{n_2}$ .

$$\mathbf{M}_{i_1 i_2} = (\mathbf{u}_1)_{i_1} (\mathbf{u}_2)_{i_2}$$

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

$$\mathbf{T}_{i_1 \dots i_r} = (\mathbf{u}_1)_{i_1} \dots (\mathbf{u}_r)_{i_r}$$

# Multilinear action on tensors

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

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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  $\mathbf{M} \in \mathbb{R}^{m_1 \times m_2}$

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

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

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

# 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  $\mathbf{m}_1 \leq n_1, \dots, \mathbf{m}_r \leq n_r$  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  $\mathbf{X} \in \mathbb{R}^n$ :

$$\begin{aligned}\mathbf{X} &= \mu + \mathbf{A}\mathbf{Z} + \mathbf{E}, & \mu &\in \mathbb{R}^n, \mathbf{A} \in \mathbb{R}^{n \times m}, m \leq n, \\ \mathbf{Z} &\sim \mathbf{N}_m(\mathbf{0}, \mathbb{I}_m), & \mathbf{E} &\sim \mathbf{N}_n(\mathbf{0}, \sigma^2 \mathbb{I}_n), \quad \mathbf{Z} \perp \mathbf{E}.\end{aligned}$$

**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,  $\mathbf{Z} \perp \mathbf{E}$ .

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

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

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

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

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

# First results



# Spectrum of $\Sigma$

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  $\mathbf{B}_k = \mathbf{A}_k \mathbf{A}_k^\top$ .

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

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

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

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

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

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



# Rank-1 power iteration

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Let  $\text{PAIR}(\mathbf{S}_N)$  be a sample estimator of  $\text{PAIR}(\mathbf{\Sigma})$ . 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  $\mathbf{F} : \mathbb{V} \rightarrow \mathbb{V}$ :

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

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,

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

Here:

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

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

# 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.

$\psi$  = 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  $t = 0, 1, 2, \dots$

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

**Theorem:** Under mild assumptions:  $\sin \theta_k^{(1)} \leq \frac{\psi}{\omega} \cdot \frac{\sqrt{\mathbf{m}_1 \cdots \mathbf{m}_r}}{\mathbf{c}^{(r-1)/2}}$ .

Moreover,  $\frac{|\omega - \hat{\omega}^{(1)}|}{\omega} \leq \left(\frac{\psi}{\omega}\right)^2 \frac{16 r \mathbf{m}_1 \cdots \mathbf{m}_r}{\mathbf{c}^{r-1}}$ .

# 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  $m_k$ .

**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>