

Tensor Decomposition meets Reproducing Kernel Hilbert Spaces

Tammy Kolda

Model Reduction and Surrogate Modeling La Jolla, CA

September 10, 2024

Chris Brigmar

Ilustration by

Tensor Decomp meets RKHS @ MORe 24

Collaborators (RKHS work)





Brett Larsen Databricks Mosaic Research



Alex Williams Flatiron/NYU



Anru Zhang Duke

10 Sep 2024

Not pictured: Runshi Tang (Duke)

Goal: Find Low-Rank Structure in Data



Tensors

• Tensor Decompositions

Quasi-Tensors

Quasi-Tensor Decomposition

• RKHS

Aligned versus Unaligned Data

• Experimental Results



Tensors

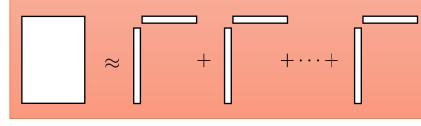
And tensor decomposition

From Matrix to Tensor Decomposition



Singular value decomposition (SVD), nonnegative matrix factorization (NMF), plus connections to Proper Orthogonal Decomposition (POD)

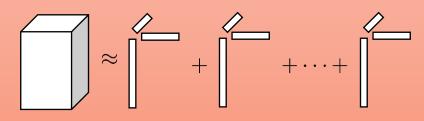
Viewpoint 1: Sum of outer products, useful for interpretation



Viewpoint 2: High-variance subspaces, useful for compression

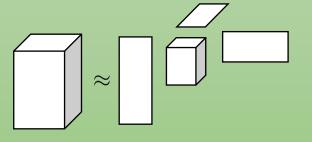


CP Model: Sum of d-way outer products, useful for interpretation



CANDECOMP, PARAFAC, Canonical Polyadic

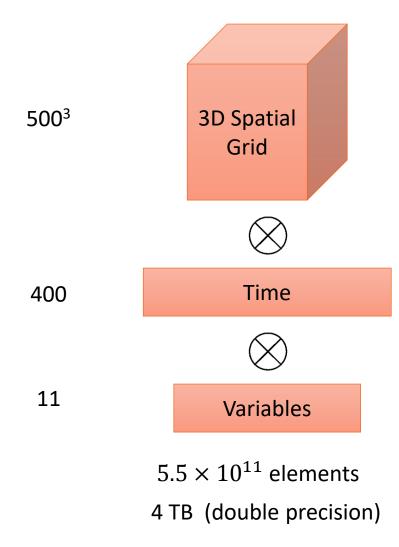
Tucker Model: Project onto high-variance subspaces to reduce dimensionality



HO-SVD, Best Rank-(R₁,R₂,...,R_d) decomposition

Other models for compression include t-SVD, tensor train, etc.

Simulations Produce Tensors!

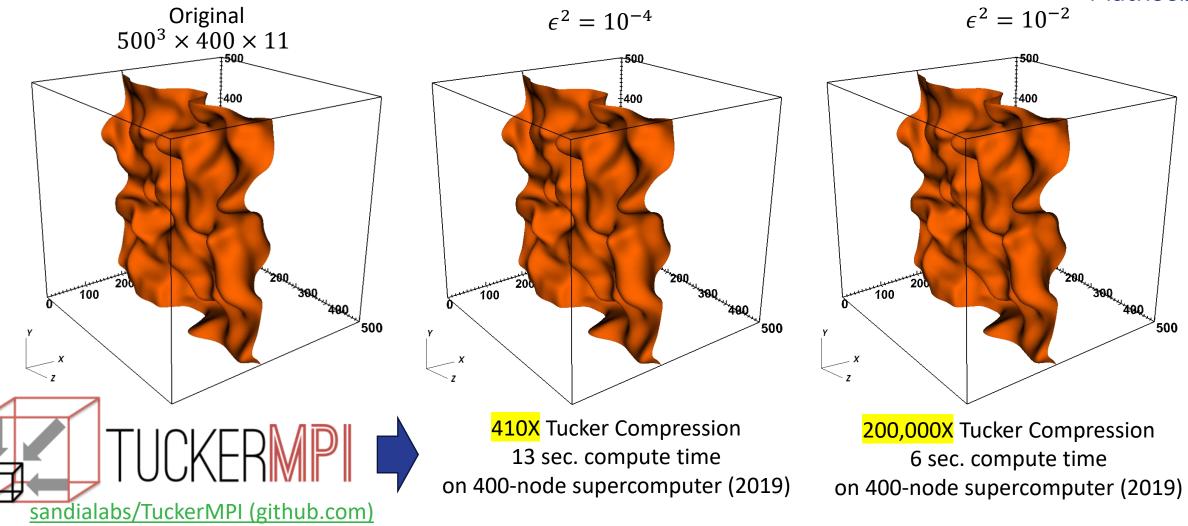


- Fluid flow DNS
 - Single computational experiment produces terabytes of data
 - Storage limits spatial, temporal resolutions
 - Difficult to analyze or transfer data
- Other applications
 - Electron Microscopy Experiments
 - Telemetry Experiments
 - Cosmology Simulations
 - Climate Modeling
- Can be compressed using tensor decompositions

MathSci.ai

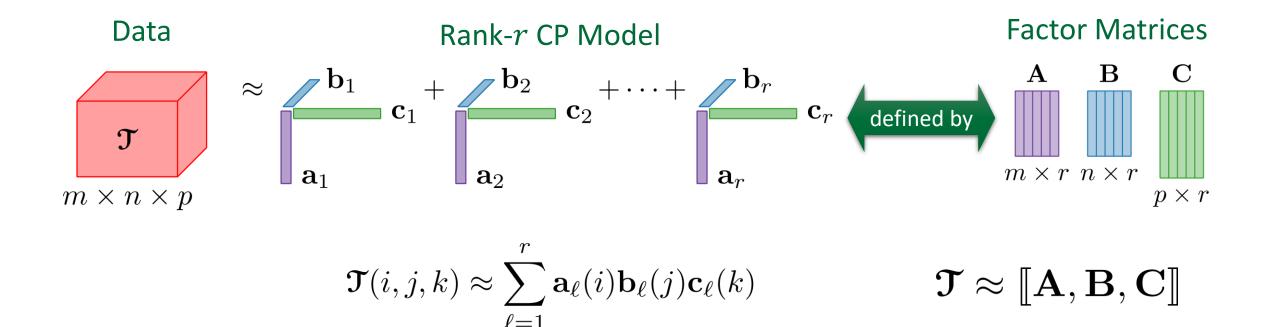
4 TB Combustion Simulation Compression





CP Tensor Decomposition



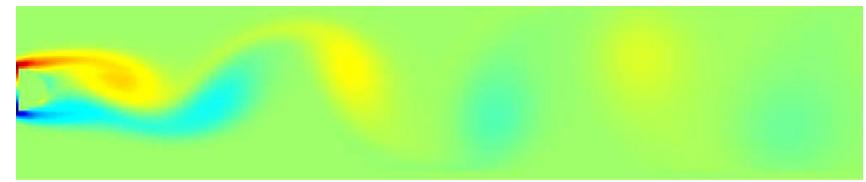


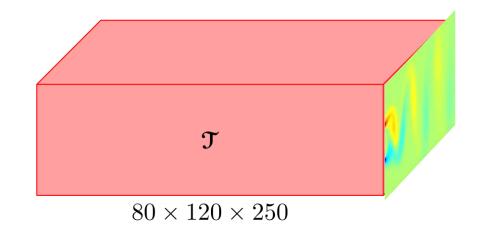
Tensor Compressed Fluid Flow Simulation



Bi-dimensional flow past a circular cylinder at Reynolds' number Re = 100

Fluid Flow Data 80 x 120 grid 250 timesteps Storage: 6×10^6 entries





Alternating Least Squares (CP-ALS)



$$\min_{\mathbf{A},\mathbf{B},\mathbf{C}} \left\| \boldsymbol{\mathfrak{T}} - [\![\mathbf{A},\mathbf{B},\mathbf{C}]\!] \right\|^2$$

$$\mathbf{\mathfrak{T}}_{m \times n \times p} \approx \mathbf{b}_{1} \mathbf{c}_{1} + \mathbf{b}_{2} \mathbf{c}_{2} + \dots + \mathbf{b}_{r} \mathbf{c}_{r}$$

1: repeat
2:
$$\mathbf{A} \leftarrow \arg\min_{\mathbf{A}} \left\| (\mathbf{C} \odot \mathbf{B}) \mathbf{A}^{\mathsf{T}} - \mathbf{T}_{(1)}^{\mathsf{T}} \right\|^{2}$$

3: $\mathbf{B} \leftarrow \arg\min_{\mathbf{B}} \left\| (\mathbf{C} \odot \mathbf{A}) \mathbf{B}^{\mathsf{T}} - \mathbf{T}_{(2)}^{\mathsf{T}} \right\|^{2}$
4: $\mathbf{C} \leftarrow \arg\min_{\mathbf{C}} \left\| (\mathbf{B} \odot \mathbf{A}) \mathbf{C}^{\mathsf{T}} - \mathbf{T}_{(3)}^{\mathsf{T}} \right\|^{2}$
5: until converged

Tensor Compressed Fluid Flow Simulation



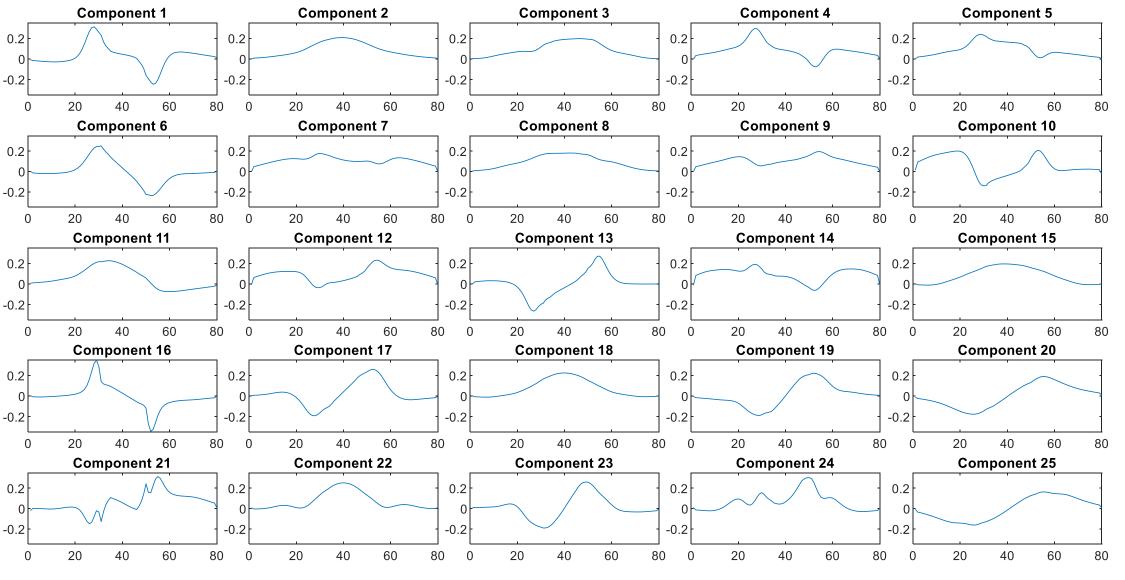
Bi-dimensional flow past a circular cylinder at Reynolds' number Re = 100

Fluid Flow Data 80 x 120 grid 250 timesteps Storage: 6 × 10⁶ entries

Tensor Compressed CP components: 25 Storage: 2×10^4 entries

Compression ratio: 400

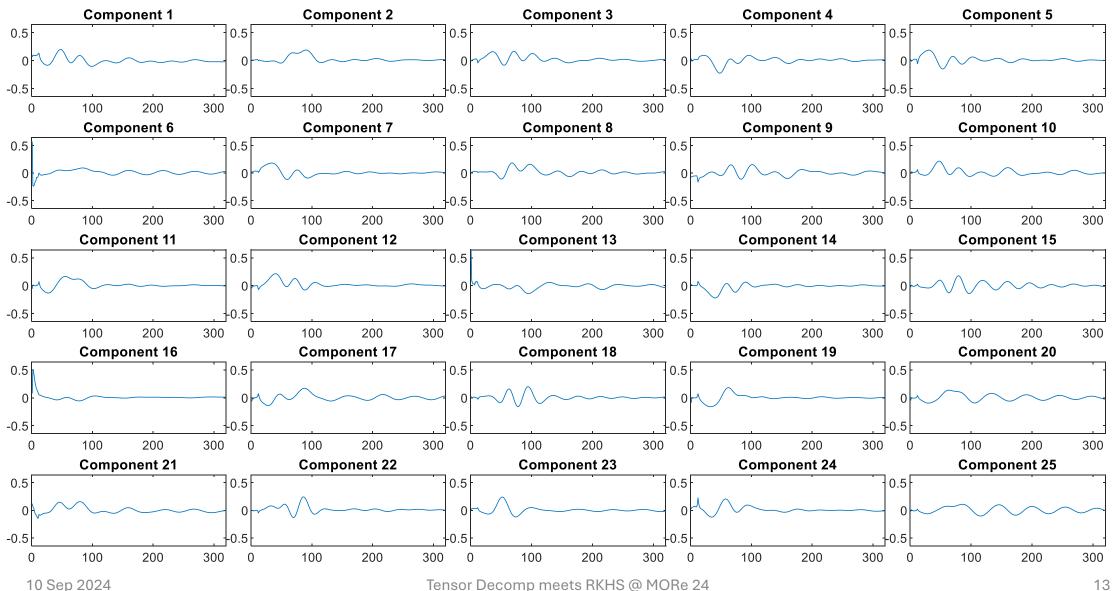
1st Spatial Mode Components

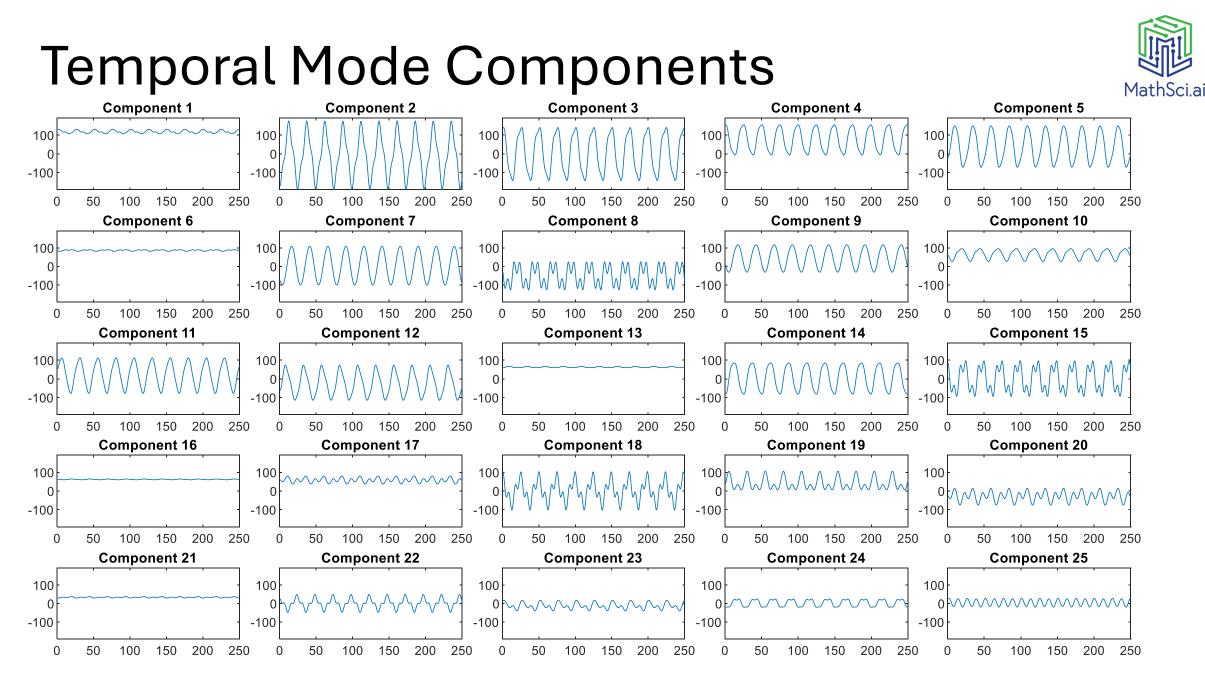


MathSci.ai

2nd Spatial Mode Components







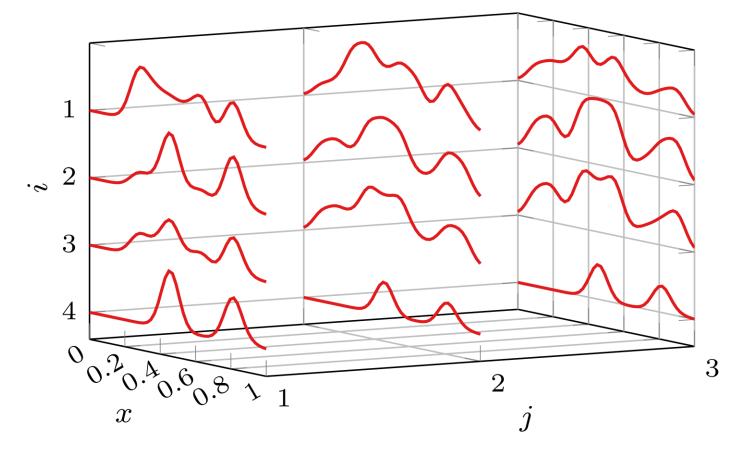


Quasi-Tensors

RKHS and quasi-tensor decomposition

Quasi-Tensor: $m \times n \times \infty$



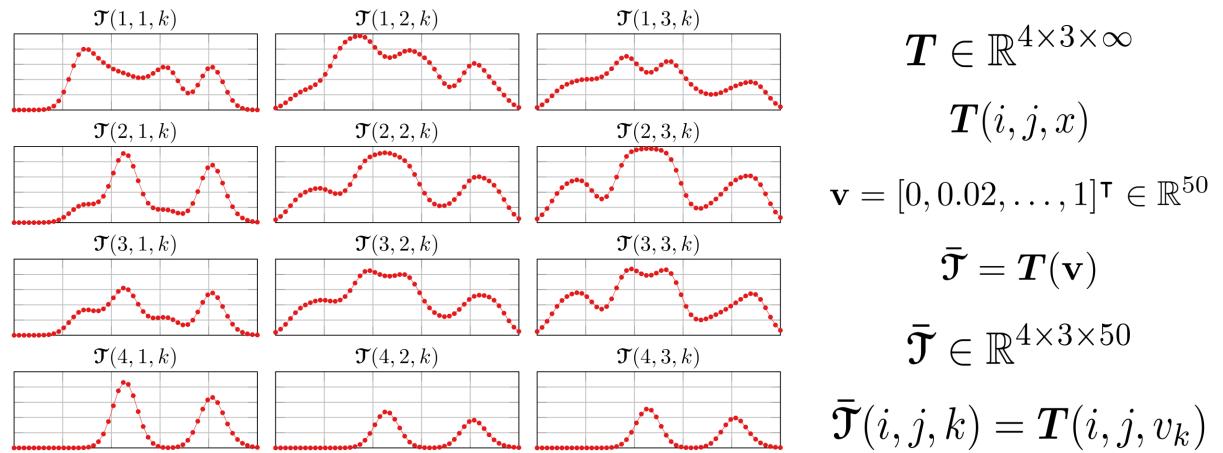


- Quasi-tensor: One or more modes of tensor are continuous
- Borrowed from quasi-matrix:
 n × ∞ array of functions
 (Townsend & Trefethen, 2014)
- Can be converted to a tensor by evaluating the functions at finitely many observations (generally only have this)
- Dynamics/smoothness can be important and may want to preserve it in some fashion

Quasi-Tensor → Tensor

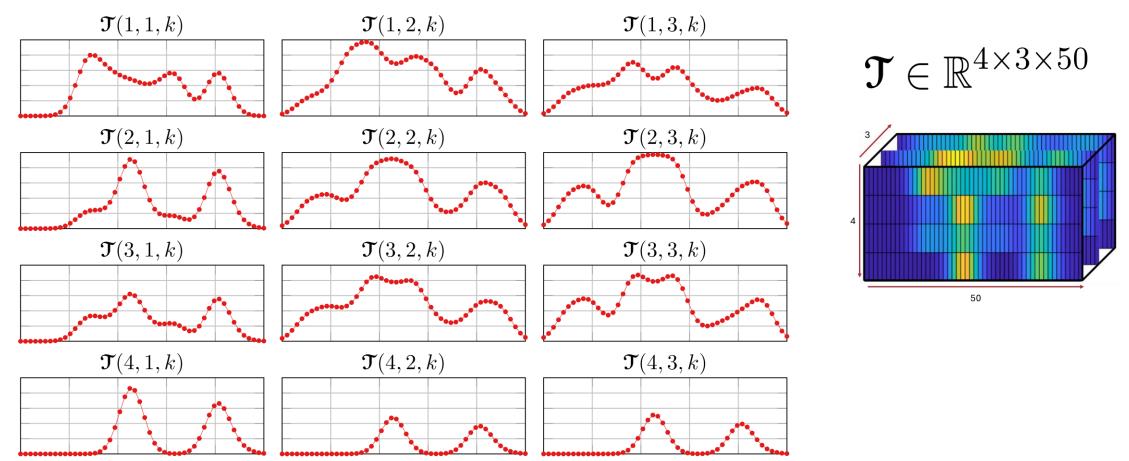
In practice, can only observe real-world quasi-tensor at discrete vales of *x*



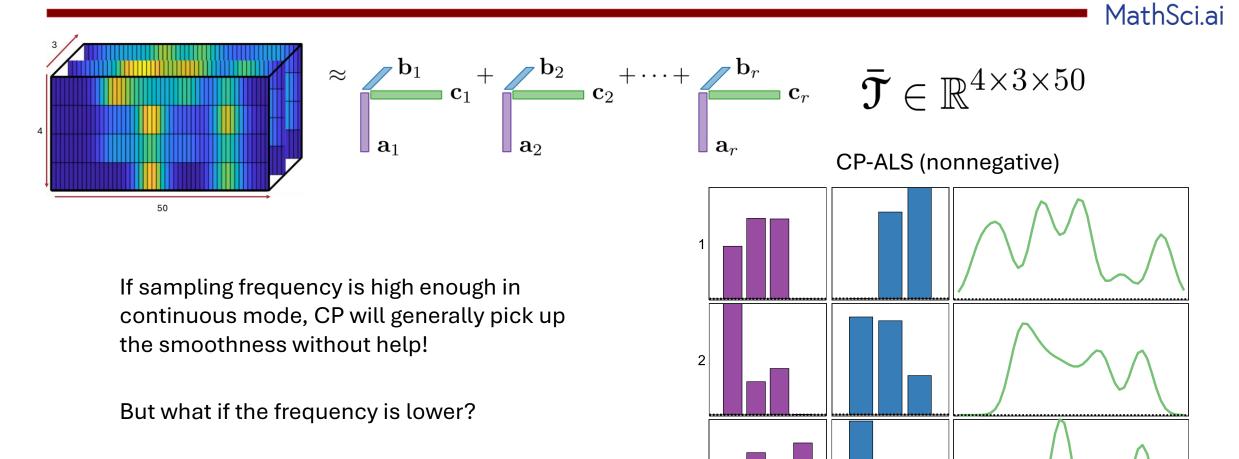


Synthetic Data Example





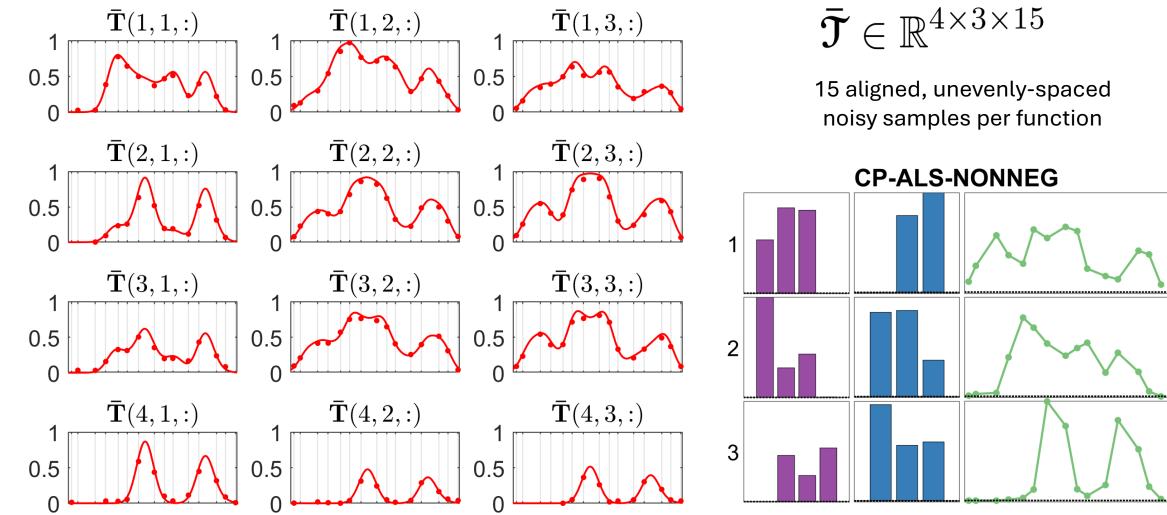
Rank-3 Factorization by CP-ALS



3

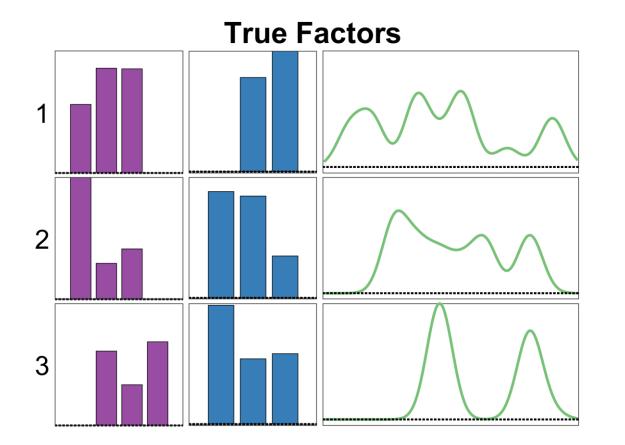
What happens with fewer observations?

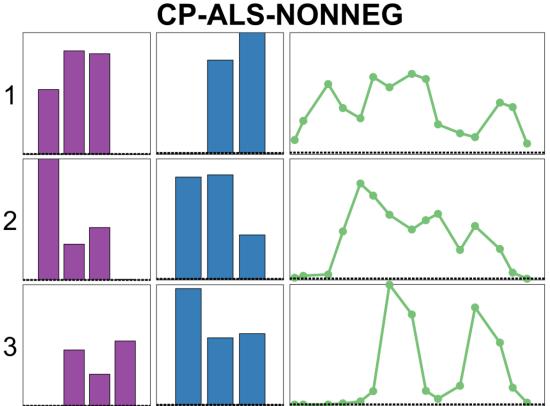




Few Observations ⇒ Jagged Components







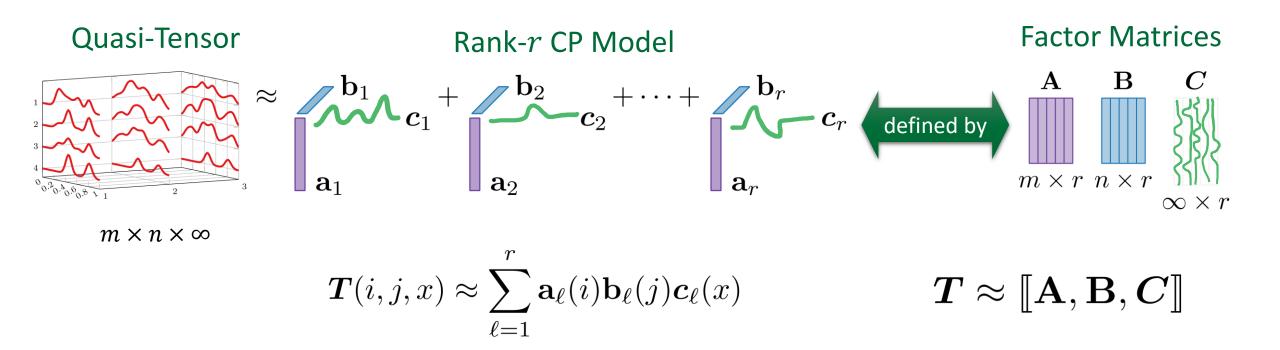


Handing Smooth Modes

CP Tensor Decomposition with Hybrid Infinite and Finite Dimensional Modes







Factors in infinite-dimensional modes are smooth functions!

10 Sep 2024

Tensor Decomp meets RKHS @ MORe 24

 $\mathbf{v} \subset \mathbb{D}^p$

 $oldsymbol{C} = egin{bmatrix} oldsymbol{c}_1 & oldsymbol{c}_2 & \cdots & oldsymbol{c}_r \end{bmatrix}$

$$\infty imes r$$

 $oldsymbol{C} \in \mathbb{R}^{\infty imes r}$

 \boldsymbol{C}

$$\boldsymbol{C}(\mathbf{v}) = \begin{bmatrix} \boldsymbol{c}_1(v_1) & \boldsymbol{c}_2(v_1) & \cdots & \boldsymbol{c}_r(v_1) \\ \boldsymbol{c}_1(v_2) & \boldsymbol{c}_2(v_2) & \cdots & \boldsymbol{c}_r(v_2) \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{c}_1(v_p) & \boldsymbol{c}_2(v_p) & \cdots & \boldsymbol{c}_r(v_p) \end{bmatrix} \in \mathbb{R}^{p \times r}$$

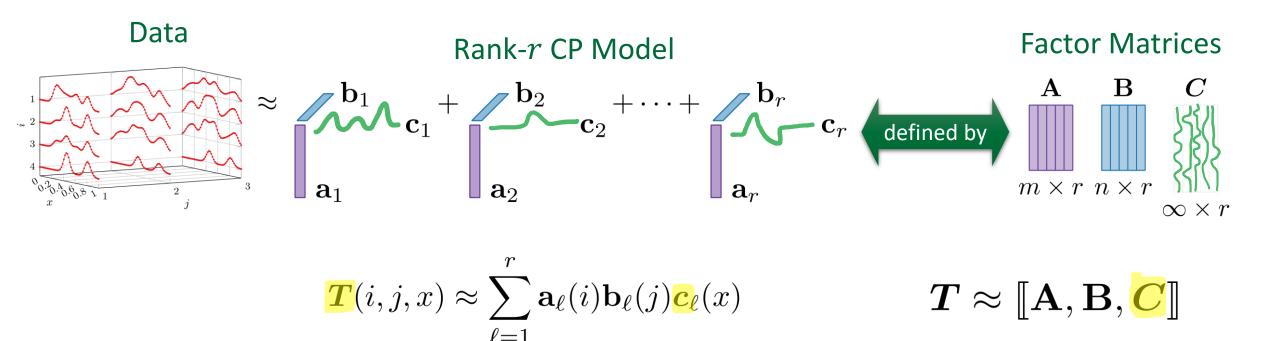
Evaluation at a vector to create matrix:

Quasi-Matrix



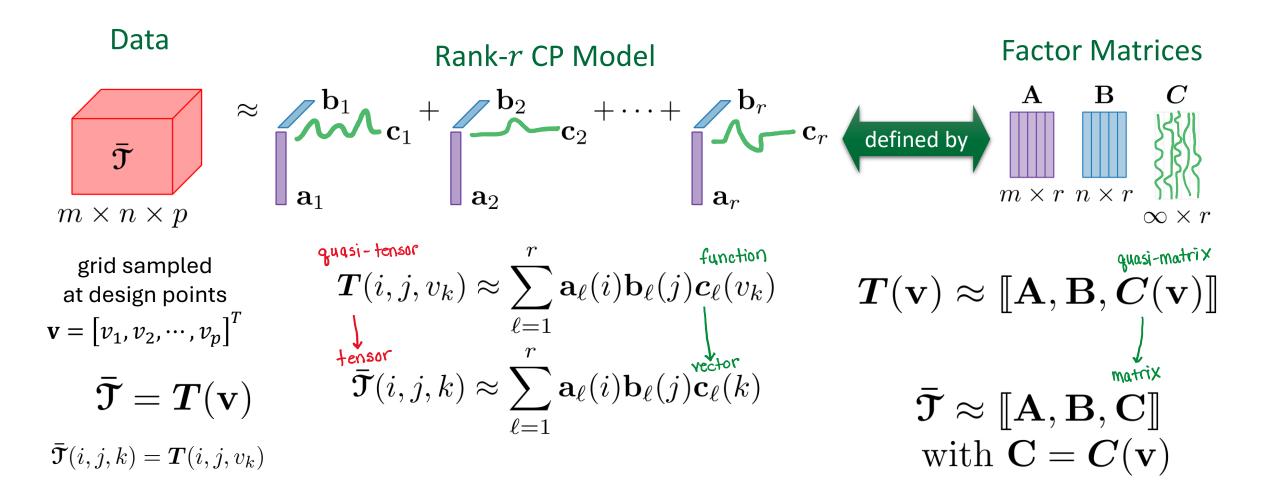
Fitting CP-HIFI Decomposition





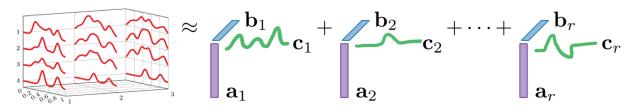
Finite-Dimensional Data





Options for Imposing Smoothness





- **C** is a matrix, but enforce smoothness
 - Linear Combination of Splines: C = SW where $S \in \mathbb{R}^{p \times q}$ is matrix of smooth b-splines and $W \in \mathbb{R}^{q \times r}$ is weight matrix (Timmerman & Kiers, 2002)
 - Second-difference Operator Regularization: $\|\mathbf{L}_2 \mathbf{C}\|^2$ where \mathbf{L}_2 is second-difference operator of size $(p-1) \times p$ (Martinez-Montes, Sanchez-Bornot, Valdes-Sosa, 2008); aka Whittaker smoothing
- C is a quasi-matrix
 - **Gaussian Process Factor Analysis** (GPFA, matrix factorization): Draws factors from an associated Gaussian process
 - Functional Principal Component Analysis (FPCA, matrix factorization): Uses Karhunen–Loeve Decomposition (i.e., continuous version of SVD)
 - **Chebfun**: linear combination of Chebyshev polynomials (matrix decomposition: Townsend & Trefethen, 2013 & 2015; Tucker decomposition: Hashemi & Trefethen, 2017)
 - **Reproducing Kernel Hilbert Space** (RKHS): Used in Tucker tensor decomposition (Han, Shi, Zhang, 2023)

•

•

kernel

Reproducing Kernel Hilbert Space (RKHS)

29

• Kernel is positive semidefinite (PSD) which means
that for any
$$\mathbf{v} = [v_1, v_2, ..., v_p]^T$$
, the matrix $\mathbf{K} \equiv \mathbf{K}(\mathbf{v}, \mathbf{v})$
is positive semidefinite

 $oldsymbol{K}(\cdot,\cdot):\mathbb{R} imes\mathbb{R} o\mathbb{R}$

Want to find smooth functions <u>but</u> impractical to

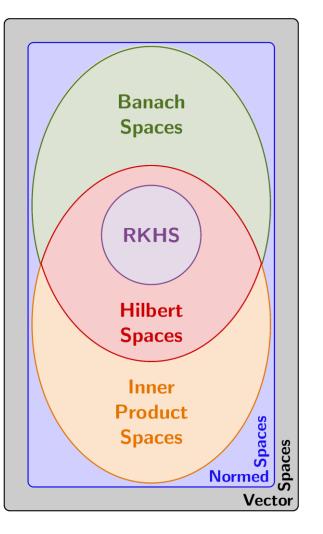
Restrict to an infinite-dimensional **Reproducing**

Kernel Hilbert Space or **RKHS** denoted as \mathcal{H}_{K} with

optimize over all functions

1)

$$\mathbf{K}(i,j) = \mathbf{K}(v_i,v_j)$$







Given a kernel:
$$oldsymbol{K}(x,y) = \exp\left(-rac{(x-y)^2}{2\sigma^2}
ight)$$

Design points: $\mathbf{v} \in \mathbb{R}^p$

Quasi-matrix: $\hat{m{K}}(\cdot) = m{K}(\cdot, \mathbf{v}) \in \mathbb{R}^{\infty imes p}$

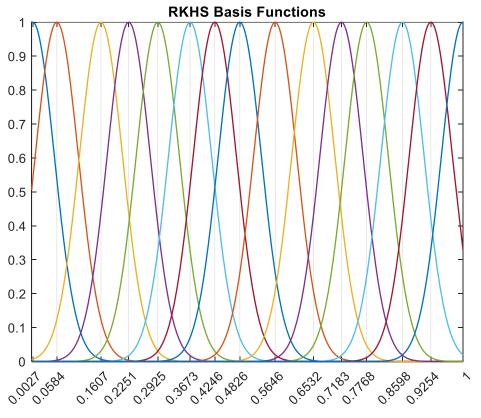
$$\hat{\boldsymbol{K}}(x) = \begin{bmatrix} \boldsymbol{K}(x, v_1) & \boldsymbol{K}(x, v_2) & \cdots & \boldsymbol{K}(x, v_p) \end{bmatrix} \in \mathbb{R}^{1 \times p}$$

Kernel Matrix:
$$\mathbf{K} = \hat{K}(\mathbf{v}) = K(\mathbf{v}, \mathbf{v}) \in \mathbb{R}^{p \times p}$$

$$\begin{bmatrix} \mathbf{K}(v_1, v_1) & \mathbf{K}(v_1, v_2) & \cdots & \mathbf{K}(v_1, v_p) \\ \mathbf{K}(v_2, v_1) & \mathbf{K}(v_2, v_2) & \cdots & \mathbf{K}(v_2, v_p) \end{bmatrix}$$

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}(v_2, v_1) & \mathbf{K}(v_2, v_2) & \cdots & \mathbf{K}(v_2, v_p) \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{K}(v_p, v_1) & \mathbf{K}(v_p, v_2) & \cdots & \mathbf{K}(v_p, v_p) \end{bmatrix} \in \mathbb{R}^{p \times p}$$

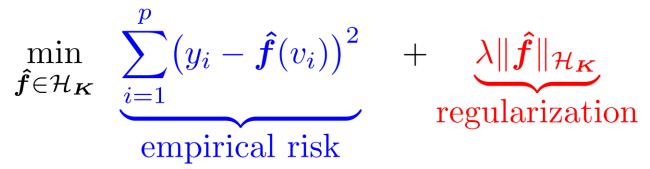




Representer Theorem Translates RKHS Problem to Finite-Dimensional Space



For a set of p observations of the form $\{v_i, y_i \equiv f(v_i)\}$ and $\lambda > 0$, we can consider the following regularized regression problem:



The **representer theorem** tells us that the optimal solution in the *infinite-dimensional Hilbert space* has the following *finite* form:

$$\hat{f}(\cdot) = \sum_{j=1}^p w_j \boldsymbol{K}(\cdot, v_j)$$

$$\hat{f}=\hat{K} \mathbf{w}$$

RKHS Problem in Practice



- Given p observations $\{v_i, y_i \equiv f(v_i)\}$
- Choose p.s.d. kernel K and regularization parameter $\lambda > 0$
- Compute $\mathbf{K}(i,j) \equiv \mathbf{K}(v_i,v_j)$
- Solve the following problem for $\mathbf{w} \in \mathbb{R}^p$:

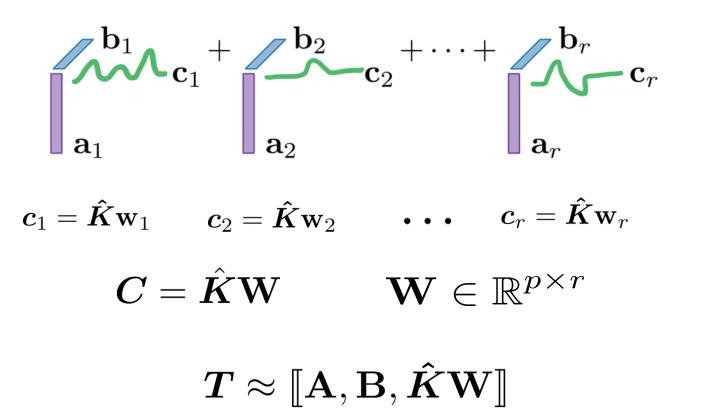
$$\min_{\mathbf{w}\in\mathbb{R}^{p}} \underbrace{\|\mathbf{K}\mathbf{w}-\mathbf{y}\|^{2}}_{\text{empirical risk}} + \underbrace{\lambda\mathbf{w}^{\mathsf{T}}\mathbf{K}\mathbf{w}}_{\text{regularization}}$$

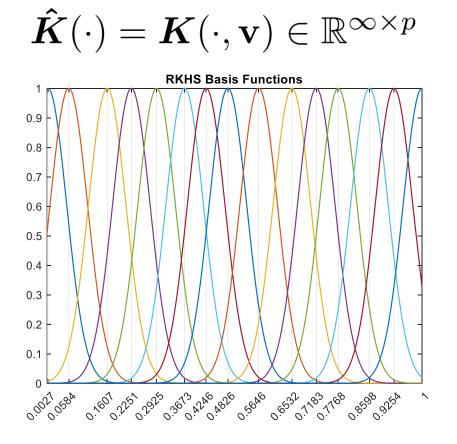
• Final solution is

$$\hat{f} = \hat{K} \mathbf{w}$$
 with $\mathbf{w} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{y}$

Representer Theorem Enables Us to Optimize in Finite-Dimensional Space

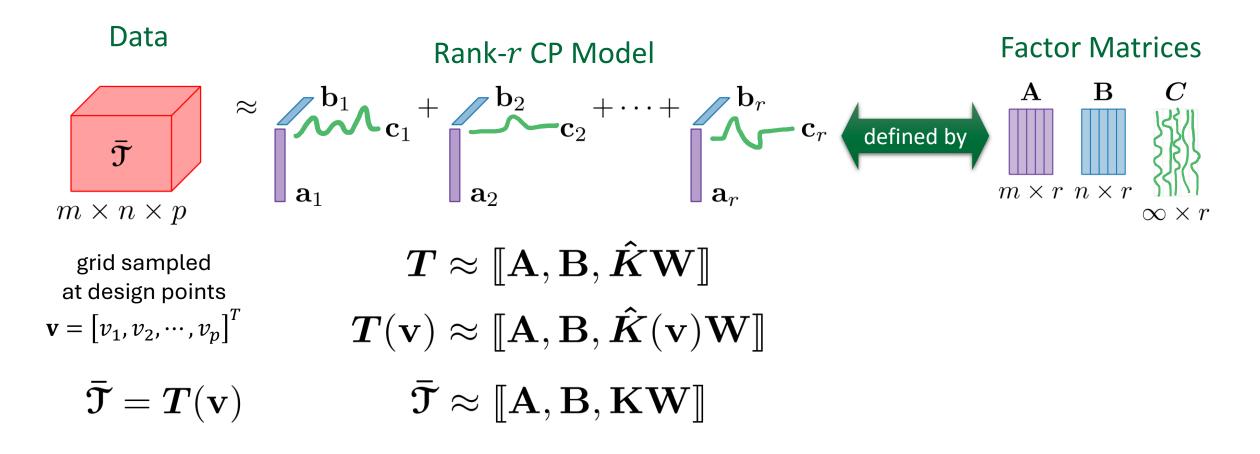






Finite-Dimensional Data





Alternating Least Squares (CP-HIFI-ALS)



$$\min_{\mathbf{A},\mathbf{B},\mathbf{W}} \left\| \bar{\boldsymbol{\mathfrak{T}}} - [\![\mathbf{A},\mathbf{B},\mathbf{KW}]\!] \right\|^2 + \lambda \|\mathbf{W}\|_{\mathbf{K}}^2$$

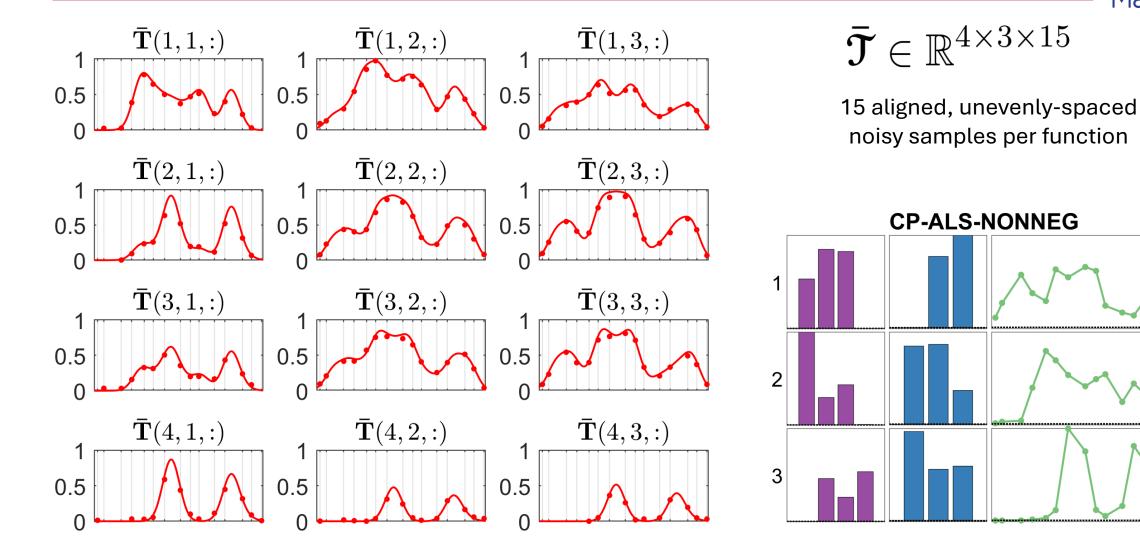
$$(\|\mathbf{W}\|_{\mathbf{K}}^2 = \sum_{j=1}^r \mathbf{w}_j^\mathsf{T} \mathbf{K} \mathbf{w}_j$$

1: repeat

- 2: $\mathbf{A} \leftarrow \arg \min_{\mathbf{A}} \| (\mathbf{KW} \odot \mathbf{B}) \mathbf{A}^{\mathsf{T}} \bar{\mathbf{T}}_{(1)}^{\mathsf{T}} \|^2$
- 3: $\mathbf{B} \leftarrow \arg\min_{\mathbf{B}} \left\| (\mathbf{KW} \odot \mathbf{A}) \mathbf{B}^{\mathsf{T}} \bar{\mathbf{T}}_{(2)}^{\mathsf{T}} \right\|^2$
- 4: $\mathbf{W} \leftarrow \arg\min_{\mathbf{W}} \left\| (\mathbf{B} \odot \mathbf{A}) \mathbf{K} \mathbf{W}^{\mathsf{T}} \bar{\mathbf{T}}_{(3)}^{\mathsf{T}} \right\|^{2} + \frac{\lambda}{2} \left\| \mathbf{W} \right\|_{\mathbf{K}}^{2}$
- 5: until converged

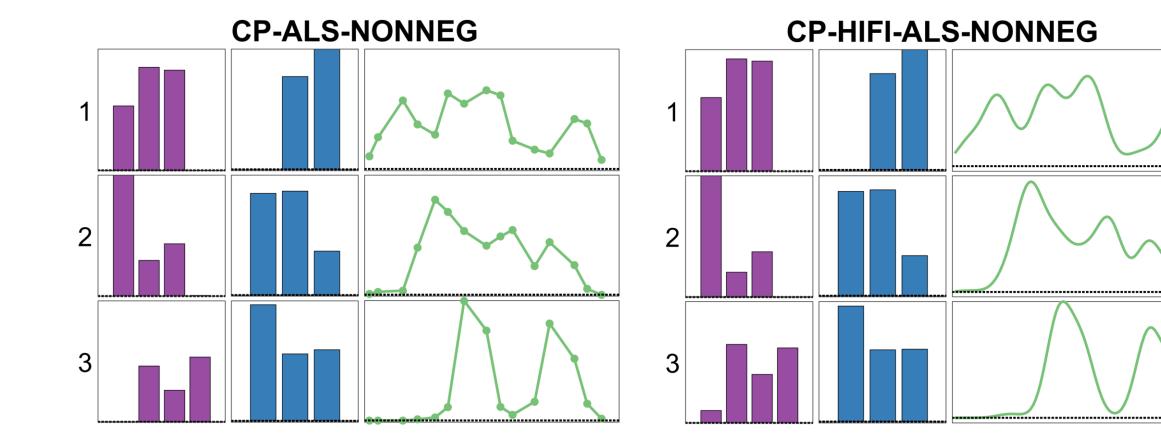
15 Aligned Observations per Function





15 Aligned Observations: CP vs CP-HIFI





10 Sep 2024

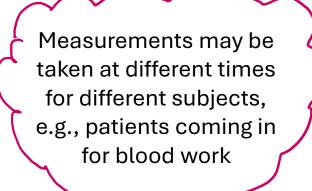


Unaligned Observations

Data Need Not Always Aligned



T(1, 1, 0.4472) = 0.4892T(4, 1, 0.5879) = 0.0262T(3, 3, 0.7482) = 0.2921T(3, 1, 0.2173) = 0.1404T(1, 3, 0.9970) = 0.0465T(3, 2, 0.8192) = 0.5155T(4, 1, 0.6799) = 0.0209T(1, 2, 0.8192) = 0.6120T(1, 1, 0.5879) = 0.5188T(4, 2, 0.2936) = 0.0025





Experimental setup may vary by site, e.g., equipment to measure weather settings might not all use same interval

Unaligned Observations

Design Points

$$\mathbf{v} = [v_1, v_2, \dots, v_p] \equiv \text{ distinct } x \text{ values in samples } T(i, j, x)$$

Observed Points

$$\Omega = \{ (i, j, k) \in [m] \otimes [n] \otimes [p] \mid \mathbf{T}(i, j, v_k) \text{ is known} \}$$

(Partially) Observed m imes n imes p Tensor

$$\bar{\boldsymbol{\mathfrak{T}}}(i,j,k) \equiv \begin{cases} \boldsymbol{T}(i,j,v_k) & \text{if } (i,j,k) \in \Omega \\ 0 & \text{if } (i,j,k) \notin \Omega \end{cases}$$

Norm on Only Observed Points

$$\|\mathbf{\mathfrak{T}}\|_{\Omega}^2\equiv\sum_{(i,j,k)\in\Omega}\mathbf{\mathfrak{T}}(i,j,k)^2$$



- T(1, 1, 0.4472) = 0.4892
- T(4, 1, 0.5879) = 0.0262
- T(3, 3, 0.7482) = 0.2921
- T(3, 1, 0.2173) = 0.1404
- $\bm{T}(1,3,0.9970)=0.0465$
- T(3, 2, 0.8192) = 0.5155
- T(4, 1, 0.6799) = 0.0209
- T(1, 2, 0.8192) = 0.6120
- T(1, 1, 0.5879) = 0.5188
- T(4, 2, 0.2936) = 0.0025



Alternating Least Squares (CP-HIFI-ALS)

$$\min_{\mathbf{A},\mathbf{B},\mathbf{W}} \left\| \bar{\boldsymbol{\mathcal{T}}} - [\![\mathbf{A},\mathbf{B},\mathbf{KW}]\!] \right\|_{\boldsymbol{\Omega}}^2 + \lambda \|\mathbf{W}\|_{\mathbf{K}}^2$$

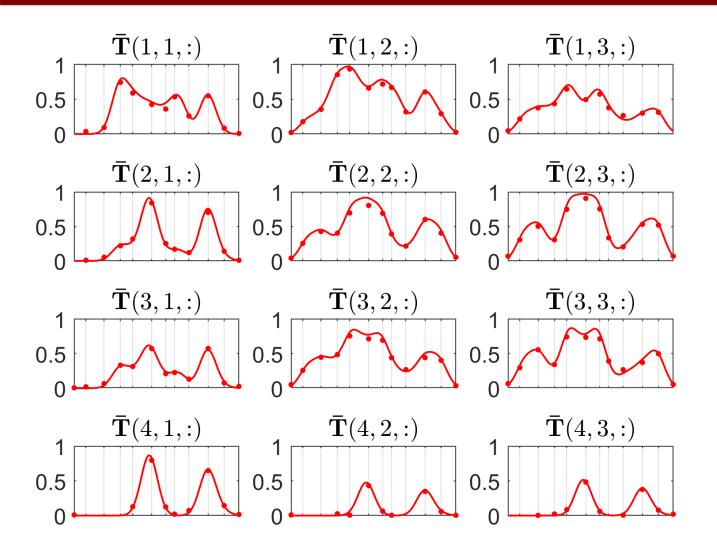
$$\begin{aligned} \|\mathbf{W}\|_{\mathbf{K}}^{2} &= \sum_{j=1}^{r} \mathbf{w}_{j}^{\mathsf{T}} \mathbf{K} \mathbf{w}_{j} \\ \|\mathbf{\mathcal{T}}\|_{\Omega}^{2} &\equiv \sum_{(i,j,k) \in \Omega} \mathbf{\mathcal{T}}(i,j,k)^{2} \end{aligned}$$

1: repeat

2:
$$\mathbf{A} \leftarrow \arg\min_{\mathbf{A}} \| (\mathbf{KW} \odot \mathbf{B}) \mathbf{A}^{\mathsf{T}} - \bar{\mathbf{T}}_{(1)}^{\mathsf{T}} \|_{\mathbf{\Omega}}^{2}$$

- 3:
- $\mathbf{B} \leftarrow \arg\min_{\mathbf{B}} \left\| (\mathbf{K}\mathbf{W} \odot \mathbf{A}) \mathbf{B}^{\mathsf{T}} \bar{\mathbf{T}}_{(2)}^{\mathsf{T}} \right\|_{\Omega}^{2}$ $\mathbf{W} \leftarrow \arg\min_{\mathbf{W}} \left\| (\mathbf{B} \odot \mathbf{A}) \mathbf{K} \mathbf{W}^{\mathsf{T}} \bar{\mathbf{T}}_{(3)}^{\mathsf{T}} \right\|_{\Omega}^{2} + \frac{\lambda}{2} \left\| \mathbf{W} \right\|_{\mathbf{K}}^{2}$ 4: 5: until converged

12 Aligned Observations per Function



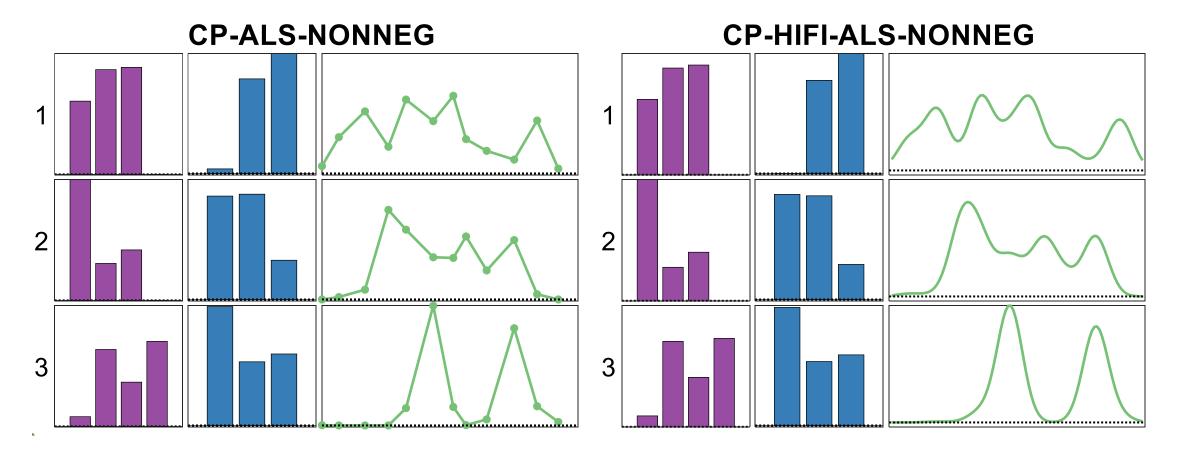
 $\bar{\mathbf{\mathfrak{I}}} \in \mathbb{R}^{4 \times 3 \times 12}$

12 aligned, unevenly-spaced

MathSci.ai

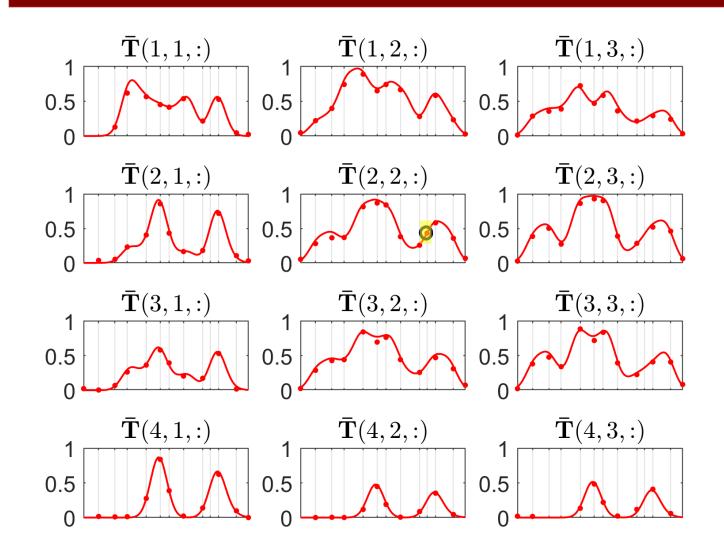
12 Aligned Observations: CP vs CP-HIFI





12 Aligned Per Function + 1 Extra Data Point



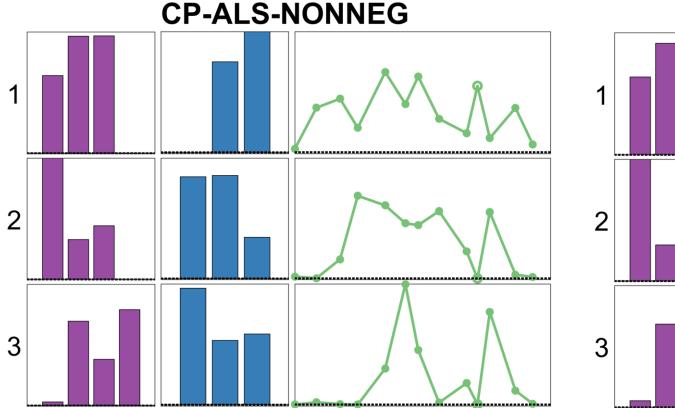


$$\mathbf{\bar{J}} \in \mathbb{R}^{4 imes 3 imes 13}$$

12 aligned, unevenly-spaced plus 1 extra point for (2,2)

12 Aligned + 1 Extra: CP vs CP-HIFI

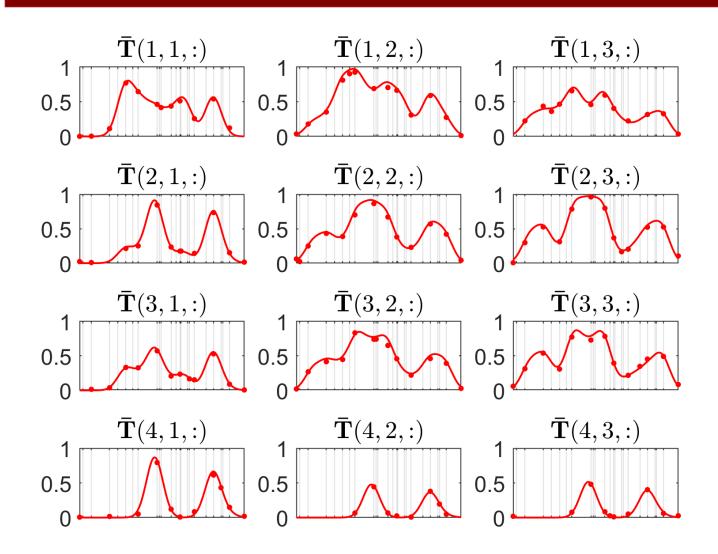




CP-HIFI-ALS-NONNEG

12 Aligned + 1 Unaligned per Function



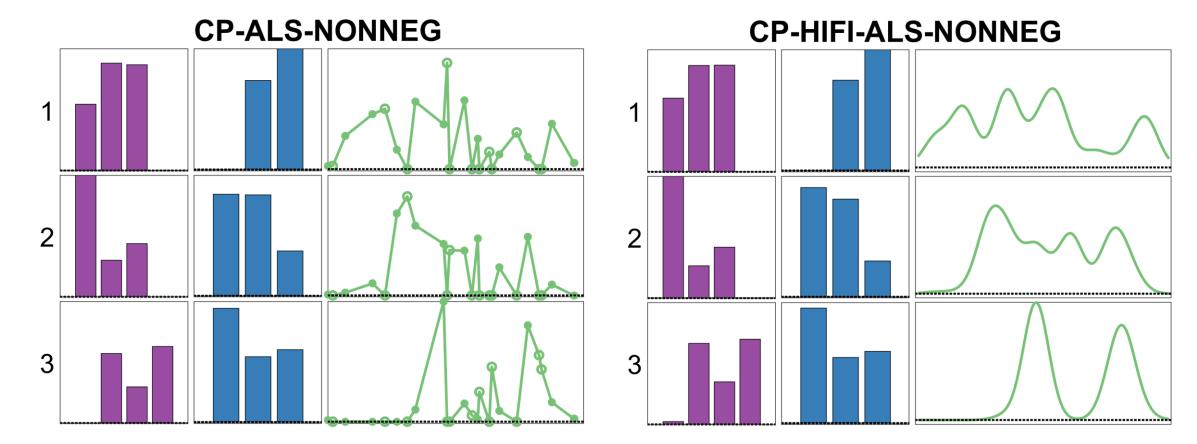


 $\bar{\mathfrak{T}} \in \mathbb{R}^{4 imes 3 imes 24}$

12 aligned, unevenly-spaced plus 1 extra point for each (i, j)

12 Aligned + 1 Unaligned: CP vs CP-HIFI

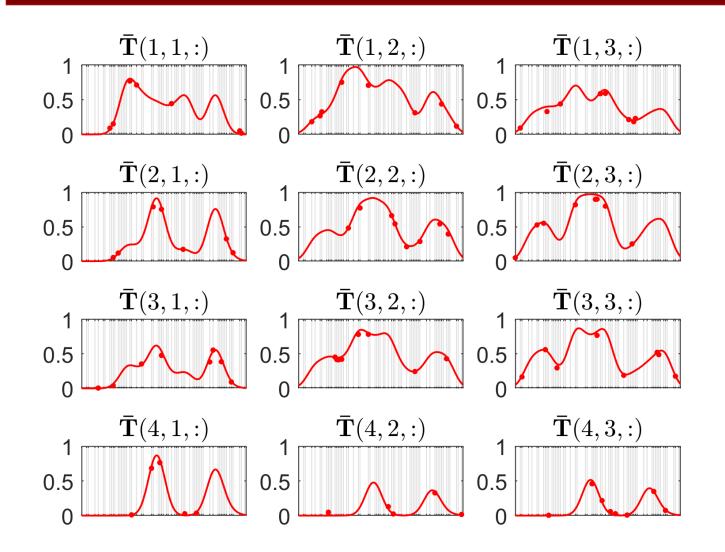




10 Sep 2024

12 Unaligned Points Per Function



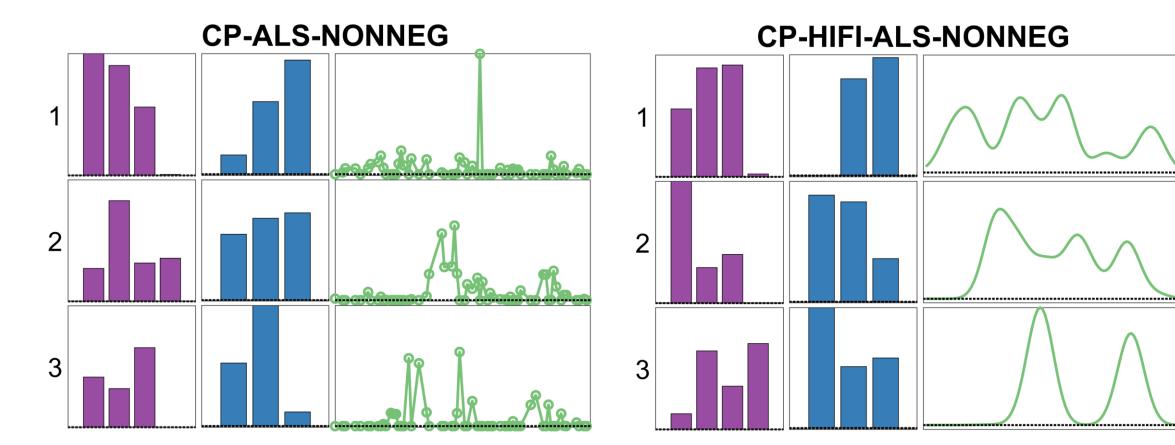


$$\mathbf{\bar{J}} \in \mathbb{R}^{4 imes 3 imes \mathbf{60}}$$

12 unaligned, unevenly-spaced points per (i, j)

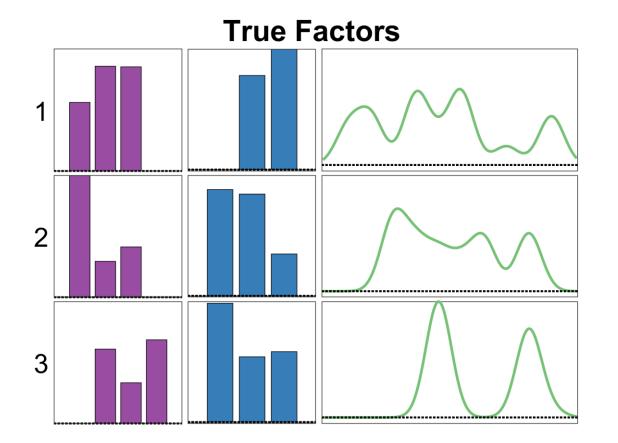
12 Unaligned: CP vs CP-HIFI



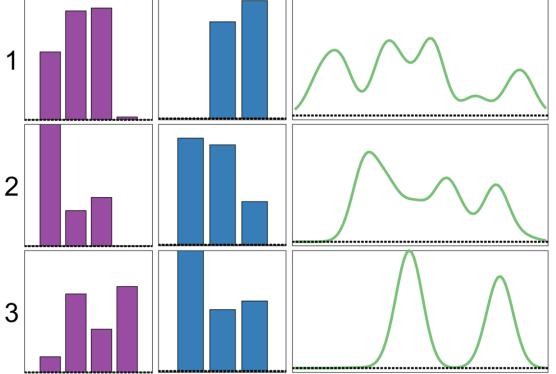


12 Unaligned: True vs CP-HIFI





CP-HIFI-ALS-NONNEG





Conclusions

Conclusions & Future Work



- Tensor data ubiquitous in modeling
- Tensor decomposition yields orders-of-magnitude reduction

Quasi-Tensors & Decomposition

- Quasi-Tensors have one or more "continuous" modes
- Decomposed with functions rather than vectors
- Variety of methods to yield functions (or function-like vectors)
- RKHS = principled way to learn smooth functions
- Aligned versus unaligned data

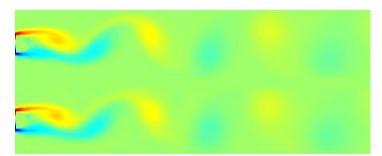
Connecting with ROM: Some Ideas...

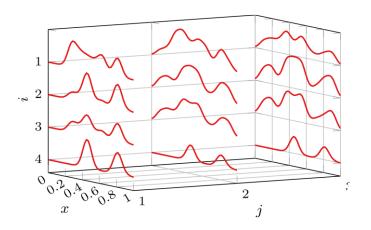
- POD with tensor rather than matrix decomposition?
- Learning functions rather than vectors (in any decomposition)?
- Assimilating unstructured grid data?

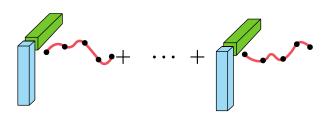


Tensor Decomposition Meets RKHS: Efficient Algorithms for Smooth and Misaligned Data, http://arxiv.org/abs/2408.05677

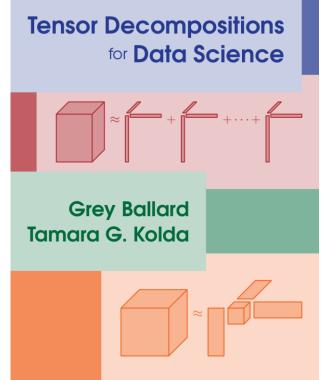






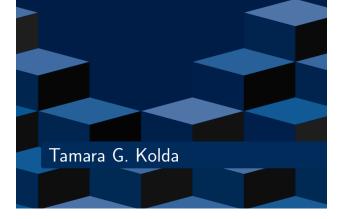


Two Books and a Channel



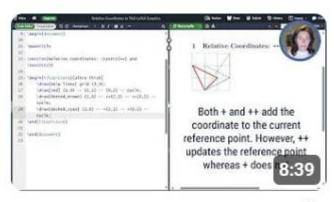
mathsci.ai/tensor-textbook PDF free online and coming soon from Cambridge University Press Unlocking IAT_EX Graphics

A Concise Guide to TikZ/PGF and PGFPLOTS



<u>latex-graphics.com</u> Print-on-demand now available and coming soon to Amazon.com Unlocking I∆T_EX Graphics

https://www.youtube.com/ @UnlockingLaTeXGraphics



Relative Coordinates (++ and +) and Turns in TikZ LaTeX...

MathSci.ai