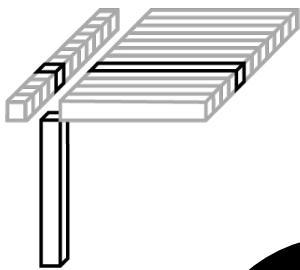


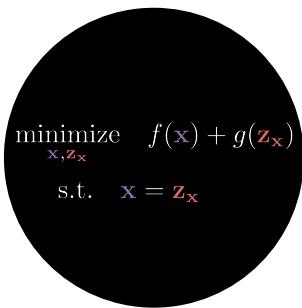
Fully Constrained PARAFAC2 with AO-ADMM

Marie Roald, Carla Schenker, Rasmus Bro, Jeremy E. Cohen, Evrim Acar
SIAM PP22 - 2022-02-25

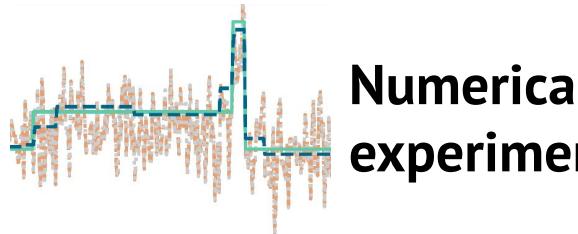
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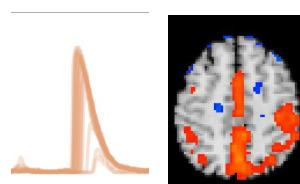
Background and motivation



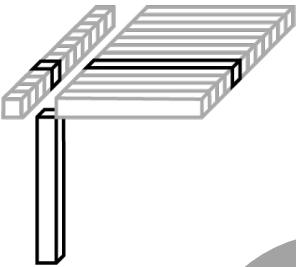
**AO-ADMM for
constraining all modes**



**Numerical
experiments**



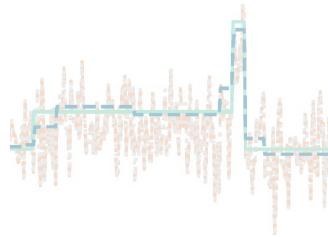
Applications



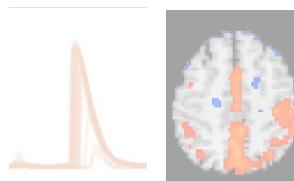
Background and motivation

$$\begin{aligned} & \text{minimize}_{\mathbf{x}, \mathbf{z}_x} f(\mathbf{x}) + g(\mathbf{z}_x) \\ & \text{s.t. } \mathbf{x} = \mathbf{z}_x \end{aligned}$$

AO-ADMM for
constraining all modes



Numerical
experiments



Applications

PARAFAC2 is a tensor decomposition method that allows the B mode to have a different factor matrix for each frontal slice

Different B factor
matrix for each mode

$$\mathbf{X}_k \approx \mathbf{A} \text{diag}(\mathbf{c}_{k:}) \mathbf{B}_k^T$$

$$\mathbf{B}_k^T \mathbf{B}_k = \Phi$$

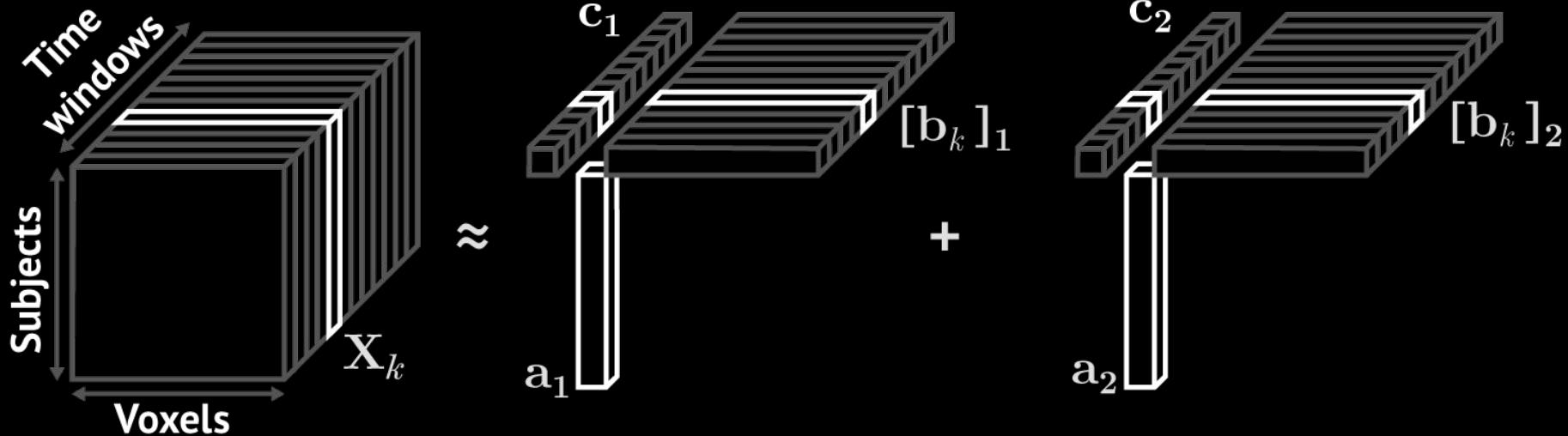
The PARAFAC2 model achieves uniqueness by imposing a constant cross product constraint on the evolving mode

$$\mathbf{X}_k \approx \mathbf{A} \text{diag}(\mathbf{c}_{k:}) \mathbf{B}_k^T$$

$$\mathbf{B}_k^T \mathbf{B}_k = \Phi$$



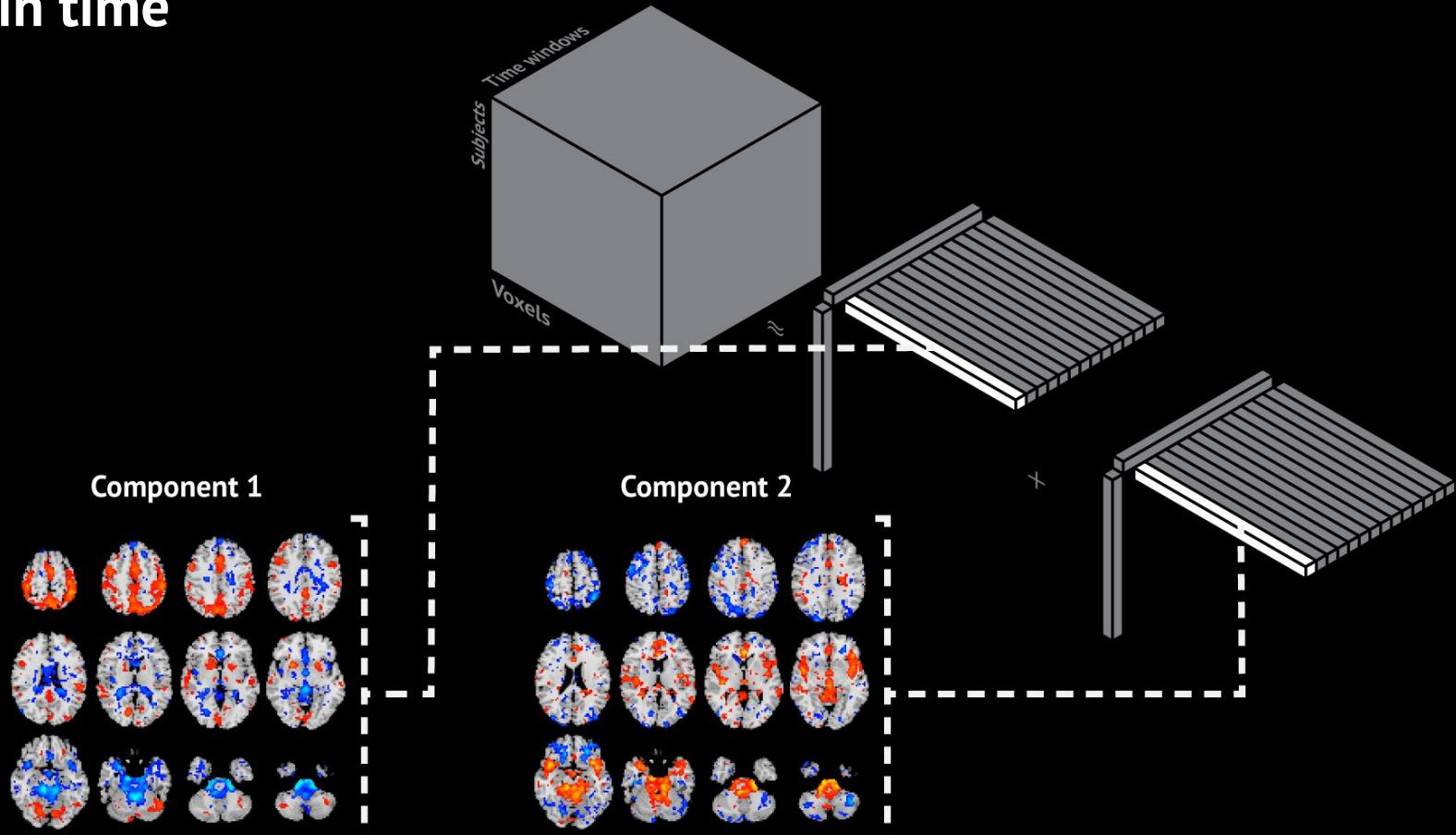
Constant cross product
for each time step



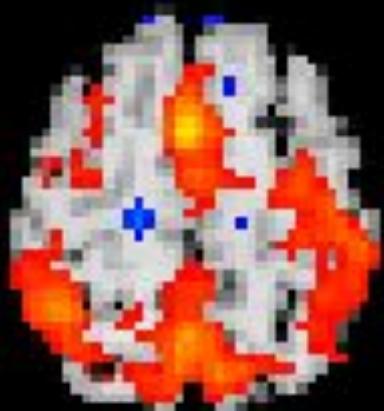
$$\mathbf{X}_k \approx \mathbf{A} \text{diag}(\mathbf{c}_{k:}) \mathbf{B}_k^T$$

$$\mathbf{B}_k^T \mathbf{B}_k = \Phi$$

PARAFAC2 captures both the meaningful components and their evolution in time



However, the PARAFAC2 model fits the noise more than the PARAFAC model and yields noisy components



Therefore we want to encourage smooth components through regularisation

To solve the PARAFAC2 problem (with Alternating Least Squares):

$$\begin{aligned} & \text{minimize}_{\mathbf{A}, \{\mathbf{B}_k, \mathbf{D}_k\}_{k \leq K}} \quad \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 \\ & \text{s.t.} \quad \mathbf{B}_k^\top \mathbf{B}_k = \Phi \quad \forall k \end{aligned}$$

To solve the PARAFAC2 problem (with Alternating Least Squares):

$$\begin{aligned} & \underset{\mathbf{A}, \{\mathbf{B}_k, \mathbf{D}_k\}_{k \leq K}}{\text{minimize}} && \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 \\ & \text{s.t.} && \mathbf{B}_k^\top \mathbf{B}_k = \Phi \quad \forall k \end{aligned}$$

We reformulate it to this problem

$$\begin{aligned} & \underset{\mathbf{A}, \Delta_B, \{\mathbf{P}_k, \mathbf{D}_k\}_{k \leq K}}{\text{minimize}} && \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k \Delta_B^\top \mathbf{P}_k^\top - \mathbf{X}_k \right\|_F^2 \\ & \text{s.t.} && \mathbf{P}_k^\top \mathbf{P}_k = \mathbf{I} \quad \forall k \end{aligned}$$

To solve the PARAFAC2 problem (with Alternating Least Squares):

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We reformulate it to this problem

$$\begin{aligned} & \underset{\mathbf{A}, \Delta_B, \{\mathbf{P}_k, \mathbf{D}_k\}_{k \leq K}}{\text{minimize}} && \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k [\Delta_B^\top \mathbf{P}_k^\top] - \mathbf{X}_k \right\|_F^2 \\ & \text{s.t.} && [\mathbf{P}_k^\top \mathbf{P}_k = \mathbf{I}] \quad \forall k \end{aligned}$$

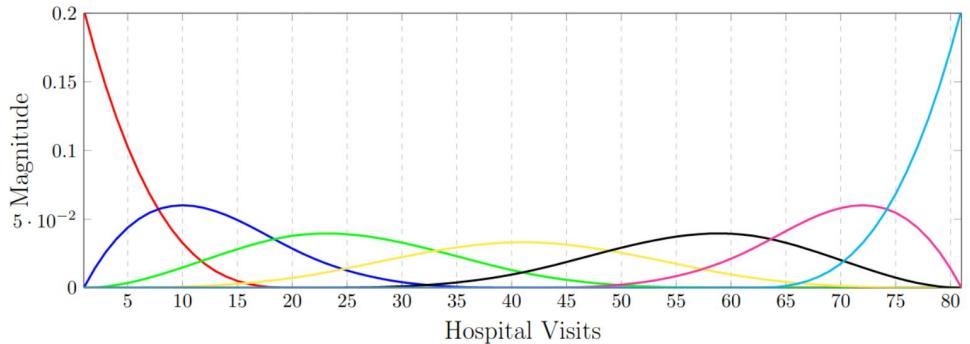
↑
Constraint

 **Evolving components**

Previous work ensures smooth components by projecting the data onto a subspace of smooth data

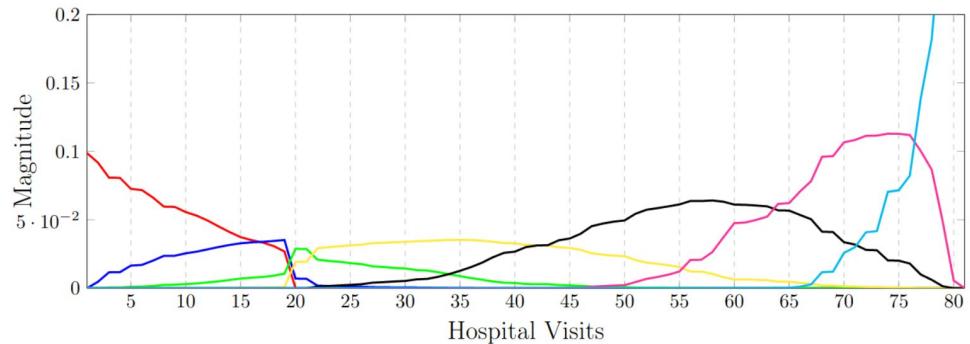
Standard B-spline basis vectors

[Helwig, N.E. Biometrical Journal 2017]



Informed M-spline basis vectors

[Afshar, A. et al. CIKM 2018]



Non-negativity has been imposed via a flexible coupling approach with HALS

$$\begin{aligned} & \underset{\mathbf{A}, \Delta_{\mathbf{B}}, \mathbf{C}, \{\mathbf{P}_k, \mathbf{B}_k\}_{k \leq K}}{\text{minimize}} \sum_{k=1}^K \|\mathbf{X}_k - \mathbf{AD}_k \mathbf{B}_k^\top\|^2 + \mu \|\mathbf{B}_k - \mathbf{P}_k \Delta_{\mathbf{B}}\|^2 \\ & \text{s.t. } \mathbf{P}_k^\top \mathbf{P}_k = \mathbf{I} \end{aligned}$$

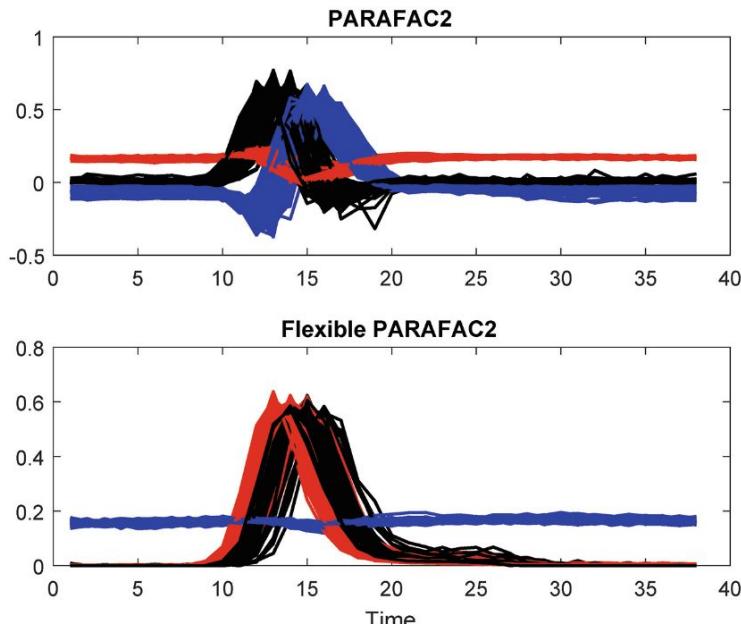
Non-negativity has been imposed via a flexible coupling approach with HALS

$$\begin{aligned} & \underset{\mathbf{A}, \Delta_{\mathbf{B}}, \mathbf{C}, \{\mathbf{P}_k, \mathbf{B}_k\}_{k \leq K}}{\text{minimize}} \sum_{k=1}^K \|\mathbf{X}_k - \mathbf{AD}_k \mathbf{B}_k^\top\|^2 + \mu \|\mathbf{B}_k - \mathbf{P}_k \Delta_{\mathbf{B}}\|^2 \\ \text{s.t. } & \mathbf{P}_k^\top \mathbf{P}_k = \mathbf{I} \end{aligned}$$

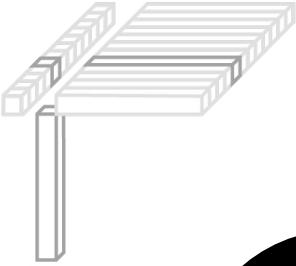


Increase every iteration
following some heuristic

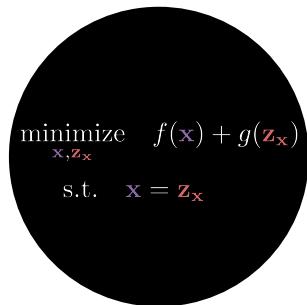
Non-negativity has been imposed via a flexible coupling approach with HALS



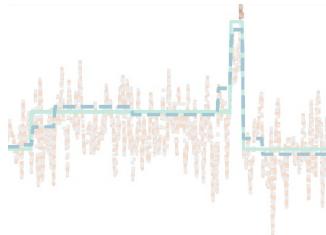
[Cohen, JE. Bro, R. LVA/ICA 2018]



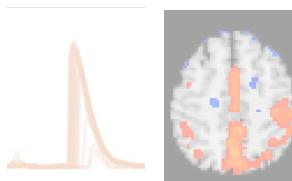
Background and motivation



AO-ADMM for constraining all modes



Numerical experiments



Applications

For the AO-ADMM scheme, we fit the modes alternately and solve the regularised subproblems with ADMM

Until convergence:

Update A matrix

Update B_k matrices

Update C matrix (D_k matrices)

The ADMM updates for the A and C matrix are well known, so we focus on how to update the B_k matrices with regularisation

Until convergence:

Update A matrix

Update B_k matrices

Update C matrix (D_k matrices)

We propose using ADMM to update the \mathbf{B}_k -components

$$\underset{\mathbf{x}}{\text{minimize}} \quad f(\mathbf{x}) + g(\mathbf{x})$$

We propose using ADMM to update the \mathbf{B}_k -components

$$\underset{\mathbf{x}, \mathbf{z}_{\mathbf{x}}}{\text{minimize}} \quad f(\mathbf{x}) + g(\mathbf{z}_{\mathbf{x}})$$

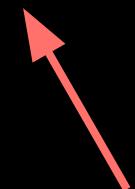


Auxiliary variable for the regularisation

We propose using ADMM to update the \mathbf{B}_k -components

$$\underset{\mathbf{x}, \mathbf{z}_{\mathbf{x}}}{\text{minimize}} \quad f(\mathbf{x}) + g(\mathbf{z}_{\mathbf{x}})$$

$$\text{s.t.} \quad \mathbf{x} = \mathbf{z}_{\mathbf{x}}$$



Auxiliary variable for the regularisation

We used the following splitting scheme to find \mathbf{B}_k -matrices with regularisation

$$\begin{aligned} & \underset{\{\mathbf{B}_k, \mathbf{Z}_{\mathbf{B}_k}, \mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}}{\text{minimize}} \quad \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) \\ \text{s.t.} \quad & \mathbf{B}_k = \mathbf{Z}_{\mathbf{B}_k}, \quad \forall k \\ & \mathbf{B}_k = \mathbf{Y}_{\mathbf{B}_k}, \quad \forall k \\ & \mathbf{Y}_{\mathbf{B}_k}^\top \mathbf{Y}_{\mathbf{B}_k} = \Phi, \quad \forall k \end{aligned}$$

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$$\begin{aligned} & \underset{\{\mathbf{B}_k, \mathbf{Z}_{\mathbf{B}_k}, \mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}}{\text{minimize}} \quad \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) \\ \text{s.t.} \quad & \mathbf{B}_k = \mathbf{Z}_{\mathbf{B}_k}, \quad \forall k \\ & \mathbf{B}_k = \mathbf{Y}_{\mathbf{B}_k}, \quad \forall k \\ & \mathbf{Y}_{\mathbf{B}_k}^\top \mathbf{Y}_{\mathbf{B}_k} = \Phi, \quad \forall k \end{aligned}$$

To obtain a problem that can be solved by ADMM, we use an implicit constraint instead of an explicit constraint for $\mathbf{Y}_{\mathbf{B}_k}$

$$\begin{aligned}
 & \underset{\{\mathbf{B}_k, \mathbf{Z}_{\mathbf{B}_k}, \mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}}{\text{minimize}} \quad \sum_{k=1}^K \left\| \mathbf{A} \mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \iota_{\text{PF2}} \left(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K} \right) \\
 \text{s.t.} \quad & \mathbf{B}_k = \mathbf{Z}_{\mathbf{B}_k}, \quad \forall k \\
 & \mathbf{B}_k = \mathbf{Y}_{\mathbf{B}_k}, \quad \forall k
 \end{aligned}$$

$$\iota_{\text{PF2}} \left(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K} \right) = \begin{cases} 0, & \text{if } \mathbf{Y}_{\mathbf{B}_k}^\top \mathbf{Y}_{\mathbf{B}_k} = \Phi \quad \forall k \\ \infty, & \text{otherwise} \end{cases}$$

Using ADMM, we obtain the following update steps:

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

Update the components to fit the data well, while still being close to the auxiliary variables

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

Update first auxiliary variable to follow regularisation while being close to the components

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

Update second auxiliary variable to follow the PF2 constraint while being close to the components

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}\left(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}\right) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

Update the first scaled dual variable to correct the regularisation coupling

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

**Update the second scaled dual variable
to correct the constraint coupling**

We repeat these steps
N times or until
convergence for every
outer iteration

$$\mathbf{B}_k^{(t+1)} \leftarrow \min_{\mathbf{B}_k} \left\{ \begin{array}{l} \left\| \mathbf{A}\mathbf{D}_k \mathbf{B}_k^\top - \mathbf{X}_k \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Z}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 + \\ \frac{\rho_k}{2} \left\| \mathbf{B}_k - (\mathbf{Y}_{\mathbf{B}_k}^{(t)} - \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2 \end{array} \right\}$$

$$\mathbf{Z}_{\mathbf{B}_k}^{(t+1)} \leftarrow \min_{\mathbf{Z}_{\mathbf{B}_k}} g_{\mathbf{B}}(\mathbf{Z}_{\mathbf{B}_k}) + \frac{\rho_k}{2} \left\| \mathbf{Z}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

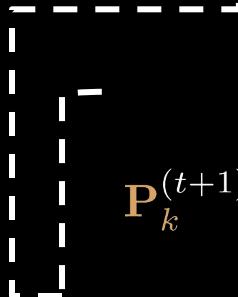
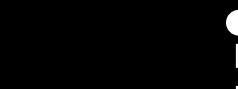
$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - (\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)}) \right\|_F^2$$

$$\boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\mathbf{Z}_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Z}_{\mathbf{B}_k}^{(t+1)}$$

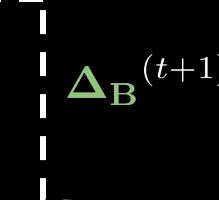
$$\boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t+1)} \leftarrow \boldsymbol{\mu}_{\Delta_{\mathbf{B}_k}}^{(t)} + \mathbf{B}_k^{(t+1)} - \mathbf{Y}_{\mathbf{B}_k}^{(t+1)}$$

To compute the update for the PARAFAC2 constraint, we use the $\mathbf{Y}_{\mathbf{B}_k} = \mathbf{P}_k \Delta_{\mathbf{B}}$ reformulation used for unconstrained PARAFAC2

$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}\left(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}\right) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \right\|_F^2$$



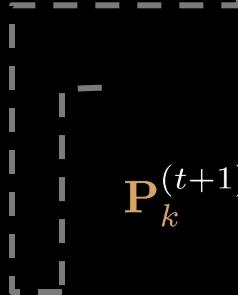
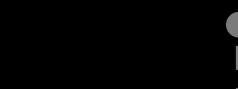
$$\mathbf{P}_k^{(t+1)} \leftarrow \mathbf{U}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top}, \quad \mathbf{U}_k^{(t+1)} \mathbf{S}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top} = \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \Delta_{\mathbf{B}}^{(t)\top}$$



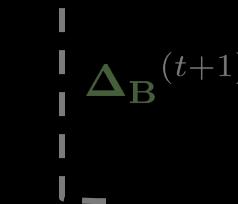
$$\Delta_{\mathbf{B}}^{(t+1)} \leftarrow \frac{1}{\sum_{k=1}^K \rho_{\mathbf{B}_k}} \sum_{k=1}^K \rho_{\mathbf{B}_k} \mathbf{P}_k^{(t+1)\top} \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right)$$

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$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}\left(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}\right) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \right\|_F^2$$



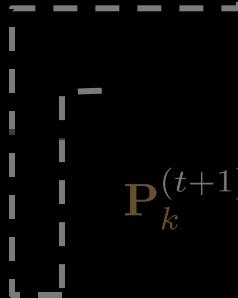
$$\mathbf{P}_k^{(t+1)} \leftarrow \mathbf{U}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top}, \quad \mathbf{U}_k^{(t+1)} \mathbf{S}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top} = \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \Delta_{\mathbf{B}}^{(t)\top}$$



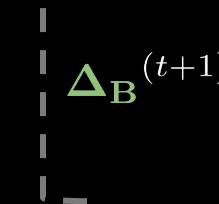
$$\Delta_{\mathbf{B}}^{(t+1)} \leftarrow \frac{1}{\sum_{k=1}^K \rho_{\mathbf{B}_k}} \sum_{k=1}^K \rho_{\mathbf{B}_k} \mathbf{P}_k^{(t+1)\top} \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right)$$

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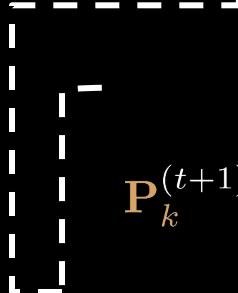
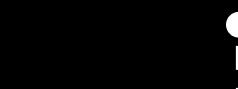
$$\mathbf{P}_k^{(t+1)} \leftarrow \mathbf{U}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top}, \quad \mathbf{U}_k^{(t+1)} \mathbf{S}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top} = \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \Delta_{\mathbf{B}}^{(t)\top}$$



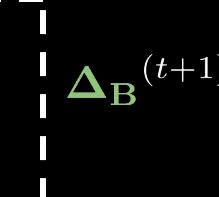
$$\Delta_{\mathbf{B}}^{(t+1)} \leftarrow \frac{1}{\sum_{k=1}^K \rho_{\mathbf{B}_k}} \sum_{k=1}^K \rho_{\mathbf{B}_k} \mathbf{P}_k^{(t+1)\top} \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right)$$

To compute the update for the PARAFAC2 constraint, we use the $\mathbf{Y}_{\mathbf{B}_k} = \mathbf{P}_k \Delta_{\mathbf{B}}$ reformulation used for unconstrained PARAFAC2

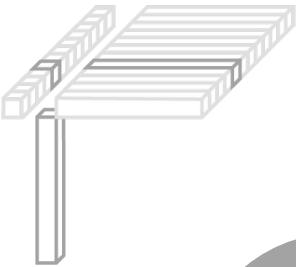
$$\{\mathbf{Y}_{\mathbf{B}_k}^{(t+1)}\}_{k \leq K} \leftarrow \min_{\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}} \iota_{\text{PF2}}\left(\{\mathbf{Y}_{\mathbf{B}_k}\}_{k \leq K}\right) + \sum_{k=1}^K \frac{\rho_k}{2} \left\| \mathbf{Y}_{\mathbf{B}_k} - \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \right\|_F^2$$



$$\mathbf{P}_k^{(t+1)} \leftarrow \mathbf{U}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top}, \quad \mathbf{U}_k^{(t+1)} \mathbf{S}_k^{(t+1)} \mathbf{V}_k^{(t+1)\top} = \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right) \Delta_{\mathbf{B}}^{(t)\top}$$



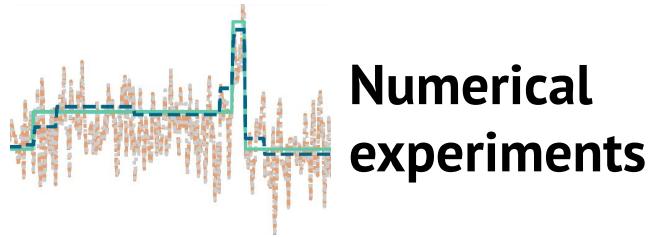
$$\Delta_{\mathbf{B}}^{(t+1)} \leftarrow \frac{1}{\sum_{k=1}^K \rho_{\mathbf{B}_k}} \sum_{k=1}^K \rho_{\mathbf{B}_k} \mathbf{P}_k^{(t+1)\top} \left(\mathbf{B}_k^{(t+1)} + \boldsymbol{\mu}_{\Delta_{\mathbf{B}, k}}^{(t)} \right)$$



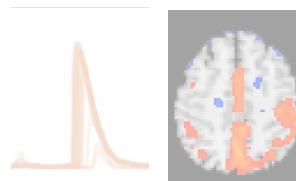
Background and motivation

$$\begin{aligned} & \text{minimize}_{\mathbf{x}, \mathbf{z}_x} f(\mathbf{x}) + g(\mathbf{z}_x) \\ & \text{s.t. } \mathbf{x} = \mathbf{z}_x \end{aligned}$$

**AO-ADMM for
constraining all modes**

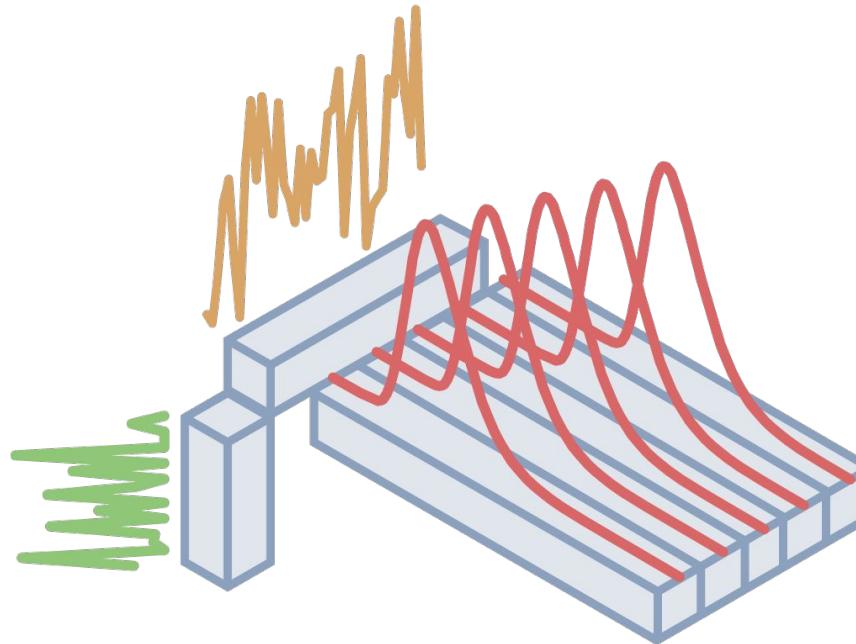


**Numerical
experiments**



Applications

To evaluate the effect of adding constraints to PARAFAC2 models with AO-ADMM, we used numerical experiments on simulated data



For evaluating unimodal constraints we generated B_k components as shifting gaussian PDFs with varying widths

A: Truncated normal ($I=10$)

B_k: PDF of Gaussian ($J=50$):

$$[b_k]_r = p_{\text{GAUSS}}(\mu_{kr}, \sigma_{kr})$$

$$\mu_{kr} \sim \mu_r + 0.41k \text{ (shifting)}$$

$$\mu_r \sim \mathcal{N}(-7, 0)$$

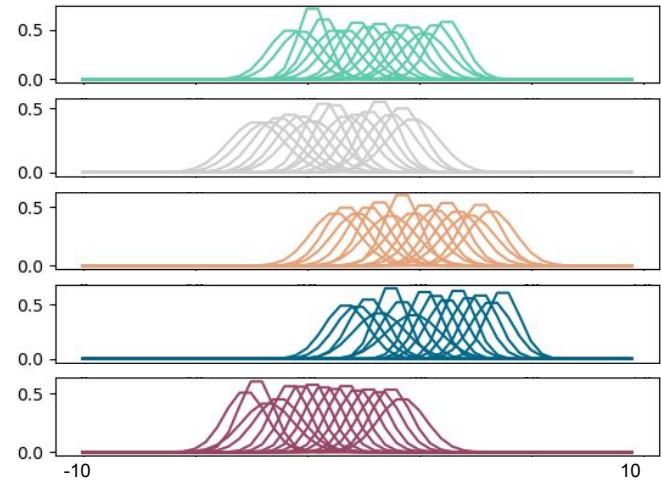
$$\sigma_{kr} \sim \sigma_r + \mathcal{N}(0, 0.1)$$

$$\sigma_r \sim U(0.5, 1)$$

C: Uniform (0.1, 1.1) ($K=50$)

η : 0.33

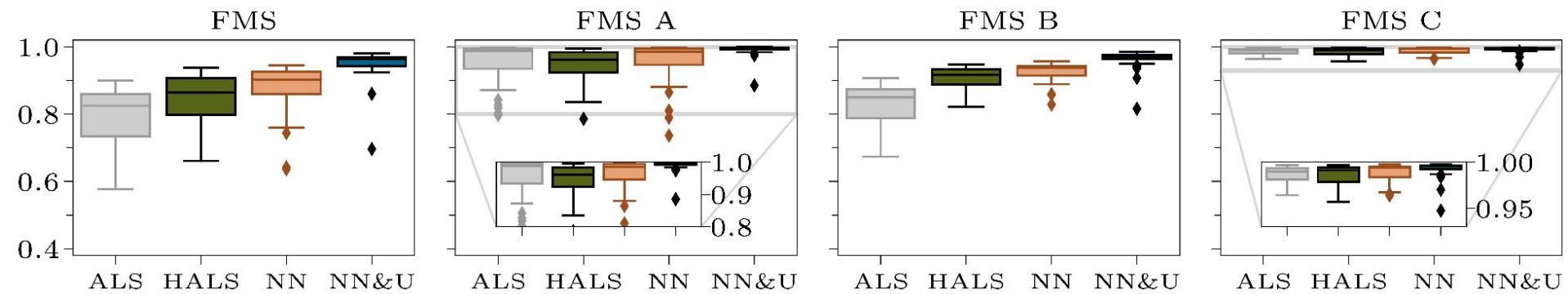
$$\mathcal{X}_{\text{noise}} = \mathcal{X} + \eta \mathcal{E} \frac{\|\mathcal{X}\|_F}{\|\mathcal{E}\|_F} \quad \mathcal{E}_{ijk} \sim \mathcal{N}(0, 1)$$



(Violates the PARAFAC2 constraint)

50 different datasets each setup, decomposed with 20 random initialisations for all models, selected model (that is not degenerate) with lowest loss.

Constraining the B_k matrices improves accuracy in all modes



ALS: Non-negative \mathbf{A} & \mathbf{C} imposed with ALS

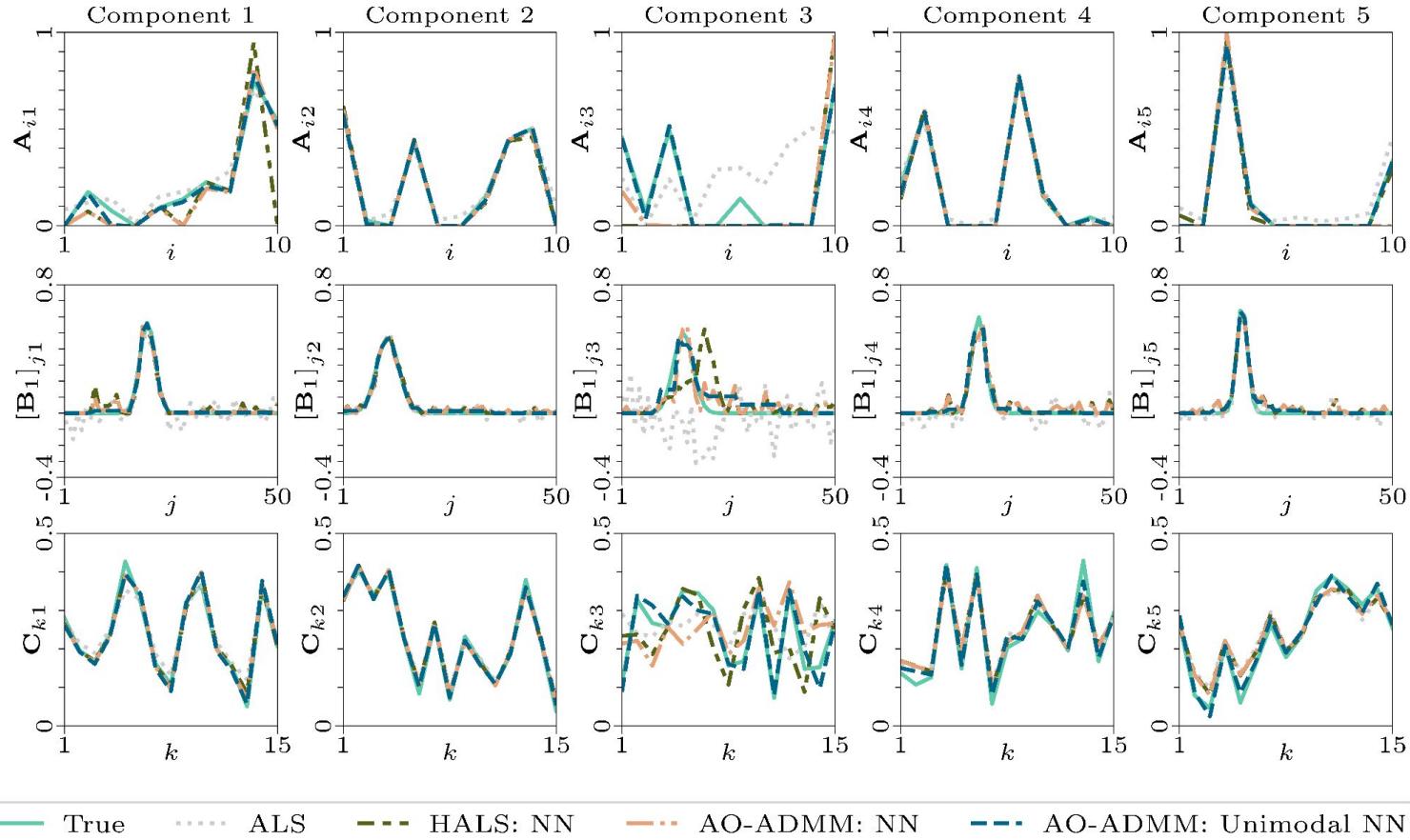
HALS: Non negative \mathbf{A} , \mathbf{B}_k s & \mathbf{C} imposed with flexible coupling with HALS

NN: Non negative \mathbf{A} , \mathbf{B}_k s & \mathbf{C} imposed with AO-ADMM

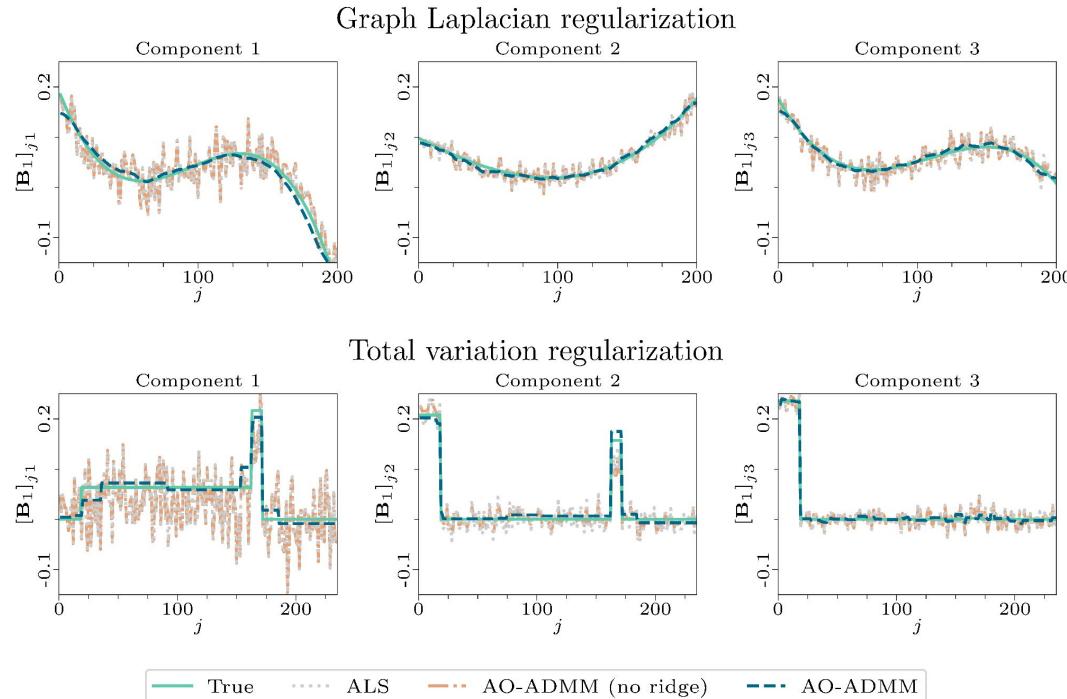
NN&U: Non negative \mathbf{A} , \mathbf{B}_k s & \mathbf{C} and unimodal \mathbf{B}_k s imposed with AO-ADMM

$$\text{FMS} = \frac{1}{R} \sum_{r=1}^R \left| \mathbf{a}_r^\top \hat{\mathbf{a}}_r \tilde{\mathbf{b}}_r^\top \hat{\mathbf{b}}_r \mathbf{c}_r^\top \hat{\mathbf{c}}_r \right|$$

Constraining the B_k matrices improves accuracy in all modes



Constrained PARAFAC2 AO-ADMM also showed improved recovery and interpretability using various other constraints



PARAFAC2 AO-ADMM is faster than the flexible coupling with HALS scheme

A: Truncated normal ($I=10$)

B_k: PDF of Gaussian ($J=50$):

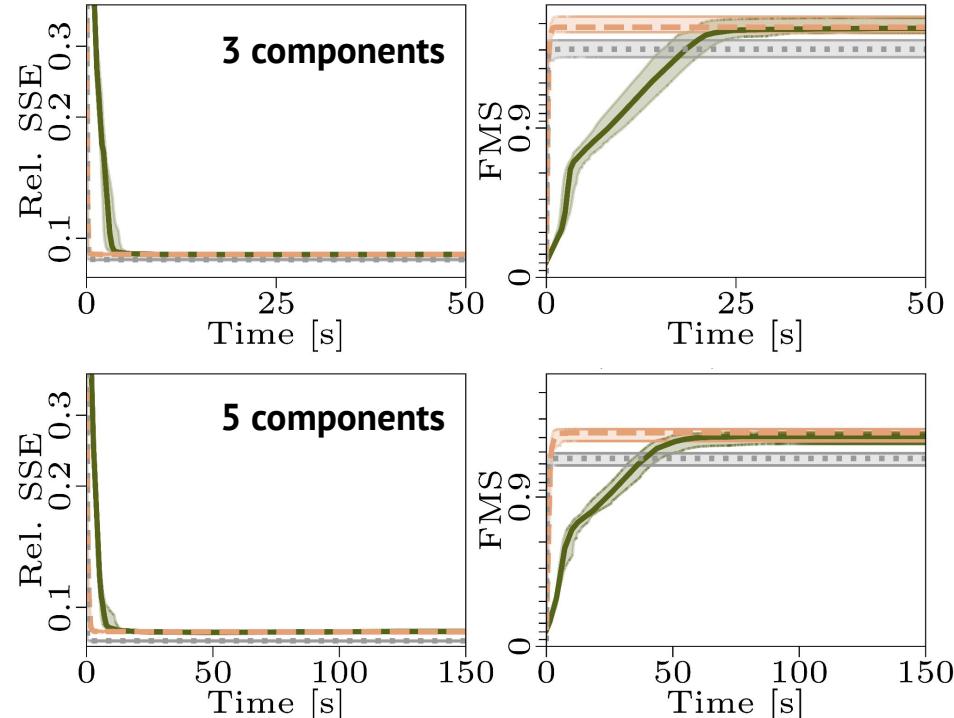
$$[b_k]_{j,r} = [b_o]_{j+k \bmod J, r}$$

[b_o]_{j,r}: Truncated normal

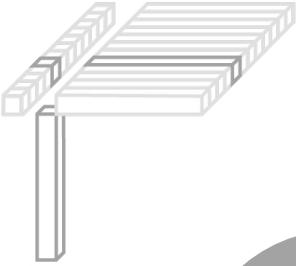
C: Uniform (0.1, 1.1) ($K=50$)

η : 0.33

$$\mathcal{X}_{\text{noise}} = \mathcal{X} + \eta \mathcal{E} \frac{\|\mathcal{X}\|_F}{\|\mathcal{E}\|_F} \quad \mathcal{E}_{ijk} \sim \mathcal{N}(0, 1)$$



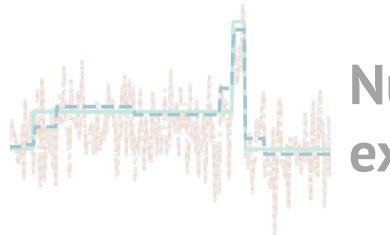
50 different datasets each setup, decomposed with 10 random initialisations for all models, selected model (that is not degenerate) with lowest loss.



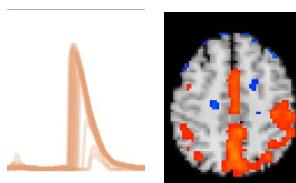
Background and motivation

$$\begin{aligned} & \text{minimize}_{\mathbf{x}, \mathbf{z}_x} f(\mathbf{x}) + g(\mathbf{z}_x) \\ & \text{s.t. } \mathbf{x} = \mathbf{z}_x \end{aligned}$$

**AO-ADMM for
constraining all modes**

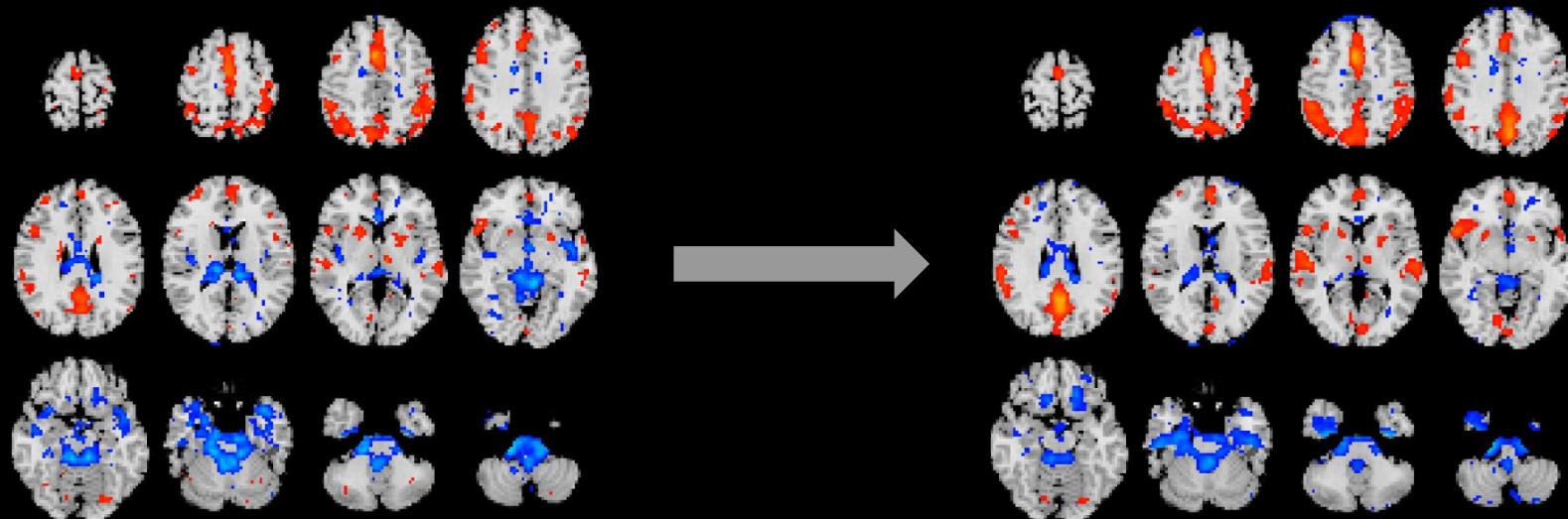


**Numerical
experiments**

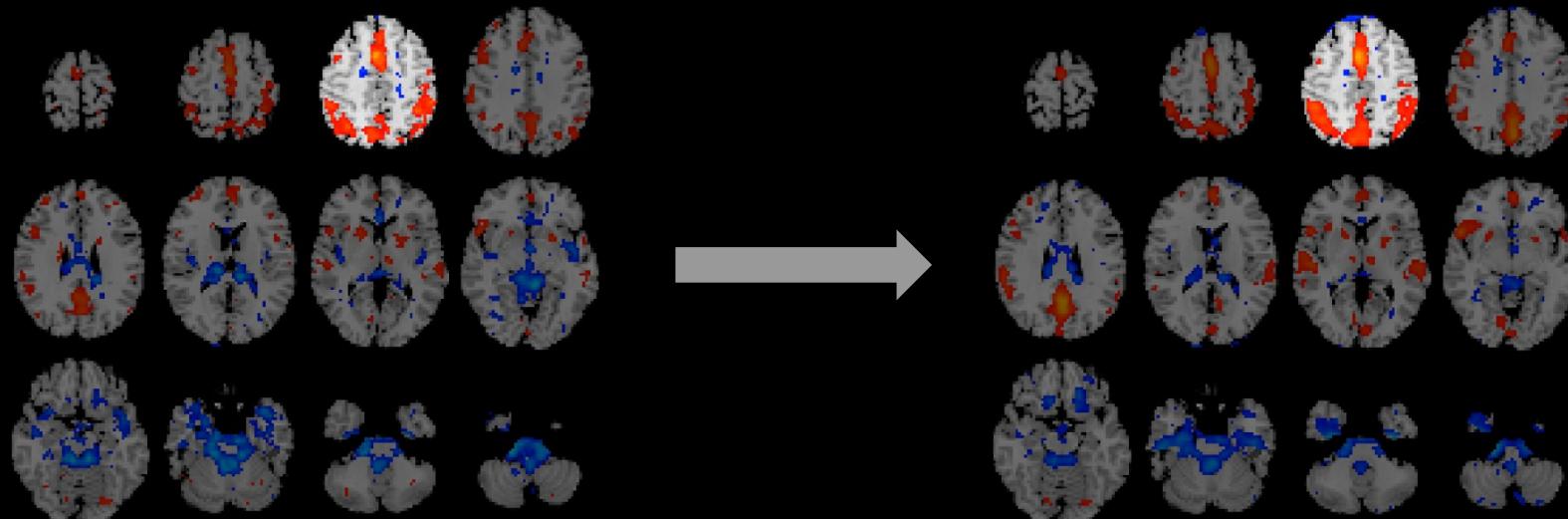


Applications

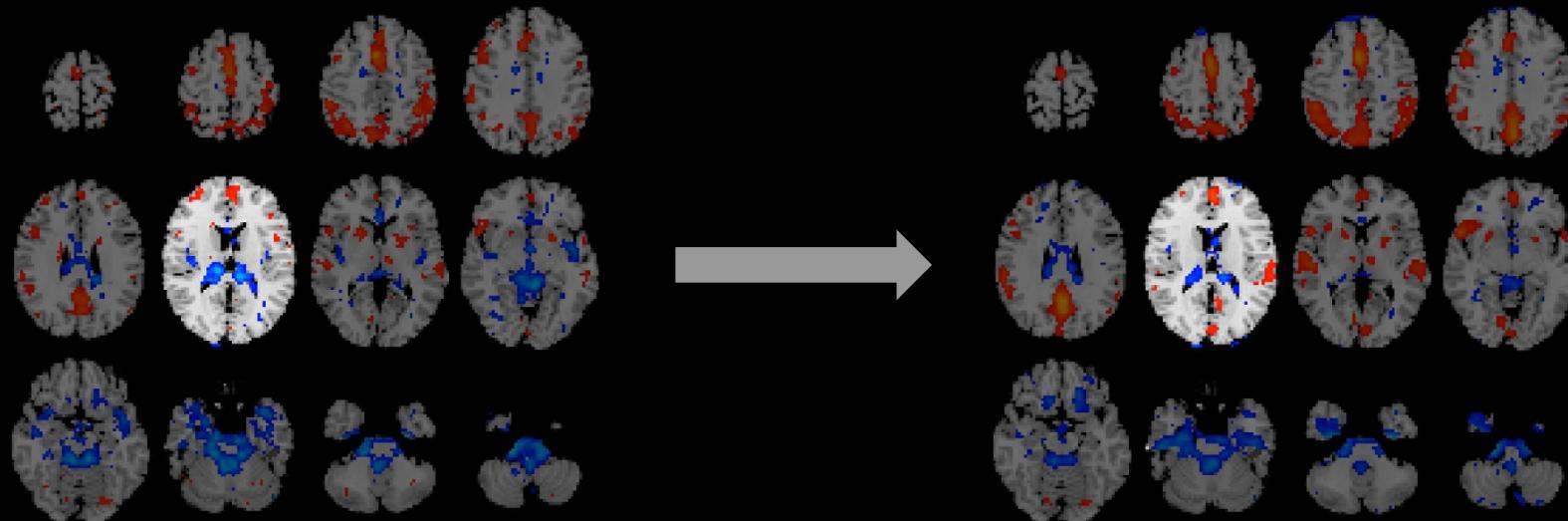
Smoothness regularisation leads to less noisy brain-activation maps when applied to fMRI data



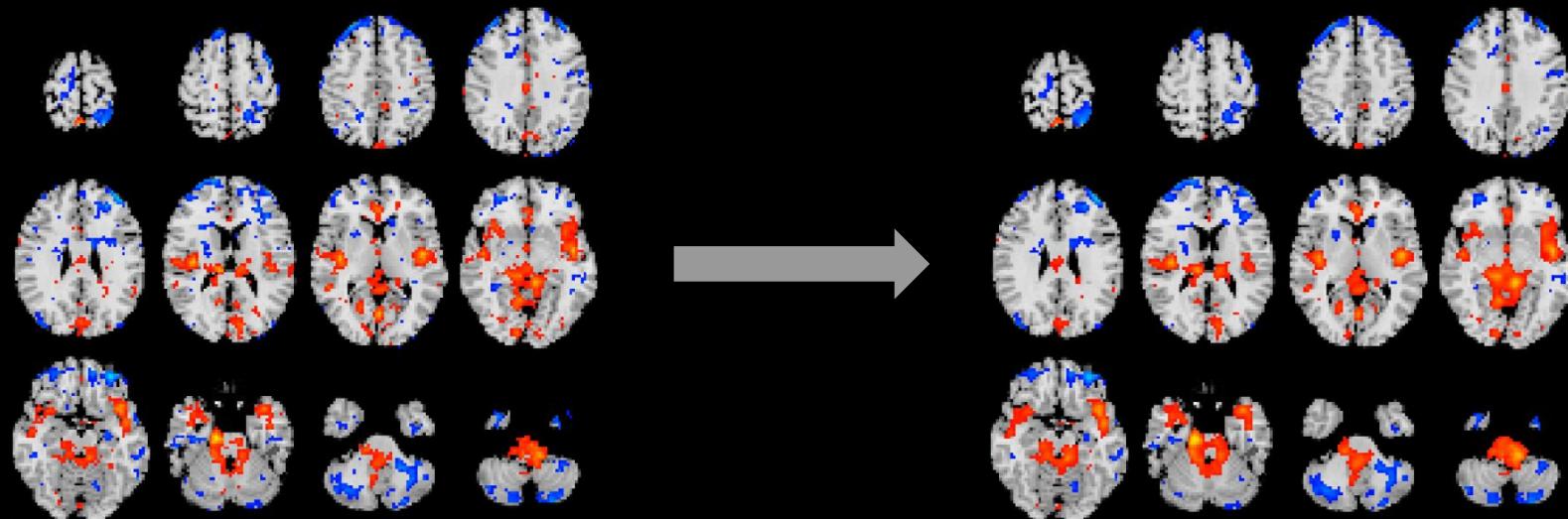
Smoothness regularisation leads to less noisy brain-activation maps when applied to fMRI data



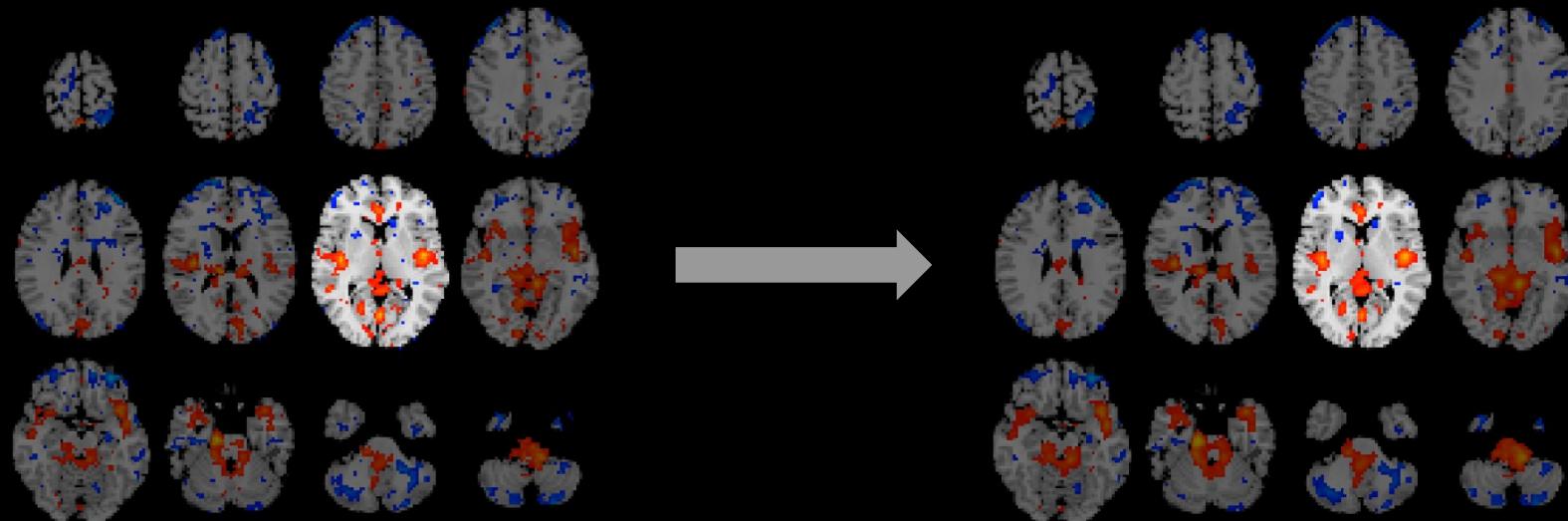
Smoothness regularisation leads to less noisy brain-activation maps when applied to fMRI data



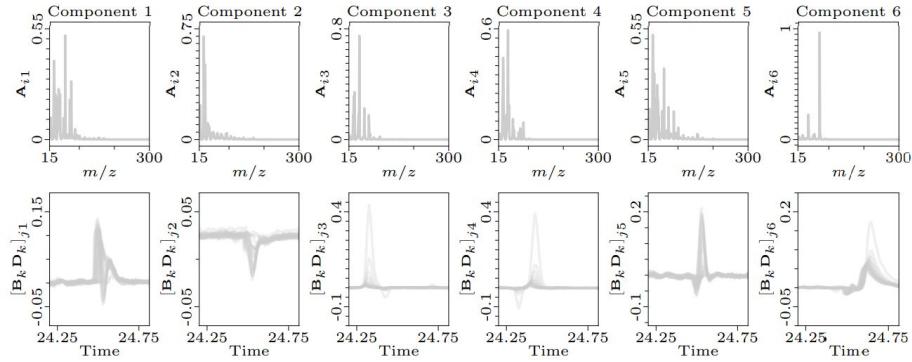
Smoothness regularisation leads to less noisy brain-activation maps when applied to fMRI data



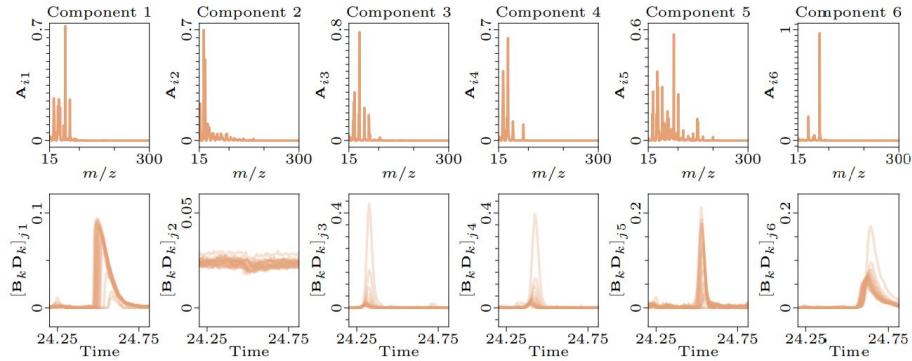
Smoothness regularisation leads to less noisy brain-activation maps when applied to fMRI data



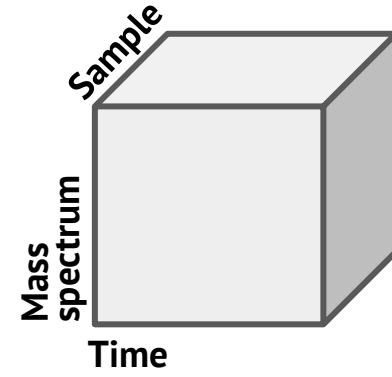
Constrained PARAFAC2 can improve interpretability in a chemometrics application



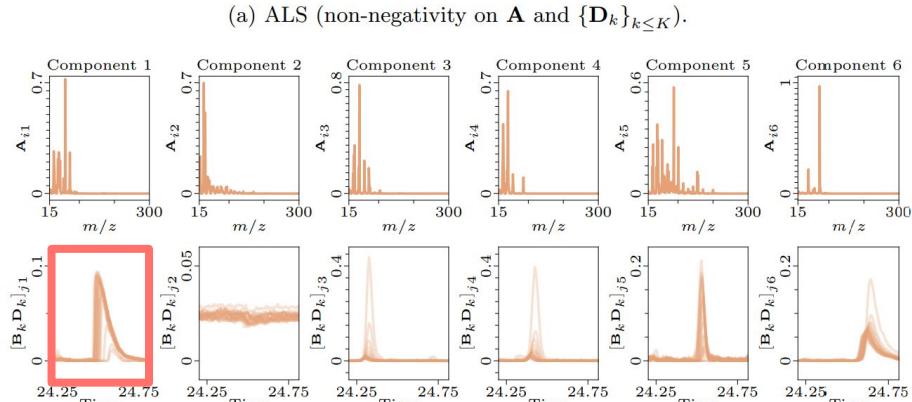
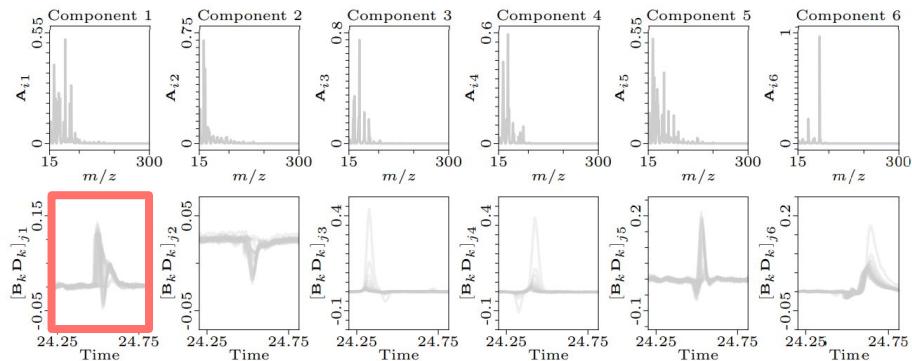
(a) ALS (non-negativity on \mathbf{A} and $\{\mathbf{D}_k\}_{k \leq K}$).



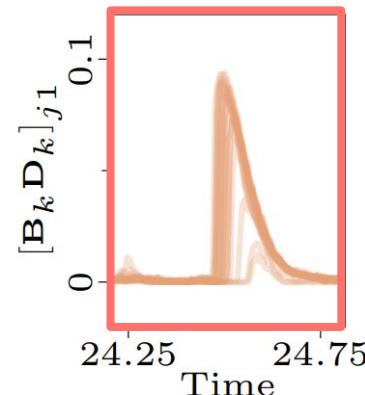
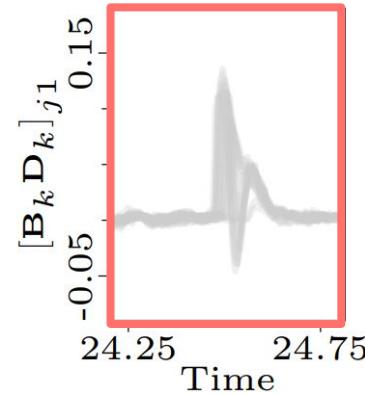
(b) AO-ADMM (non-negativity on all modes).



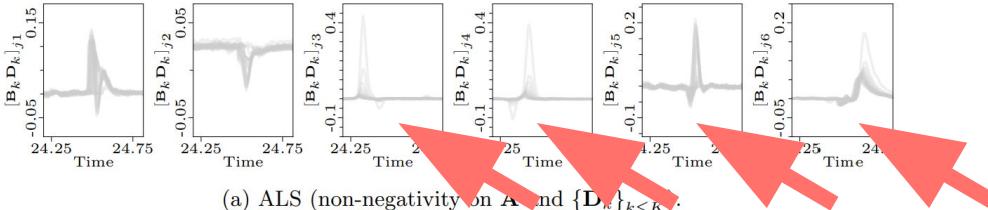
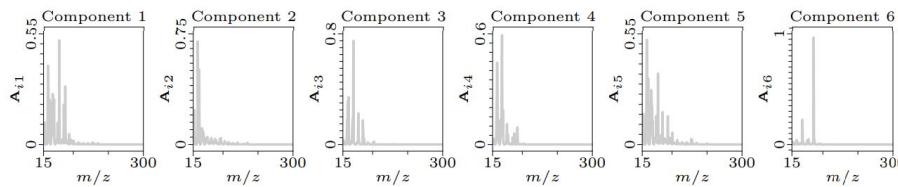
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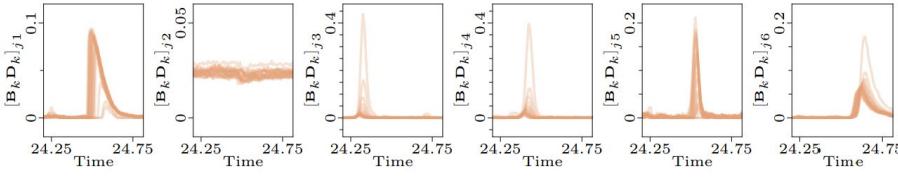
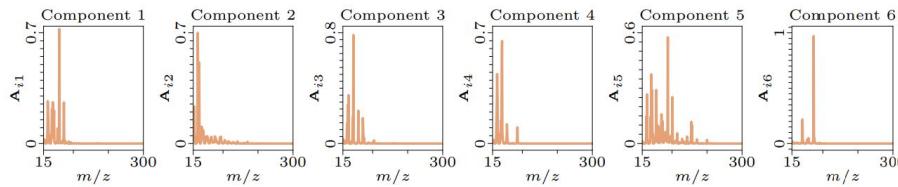
(b) AO-ADMM (non-negativity on all modes).



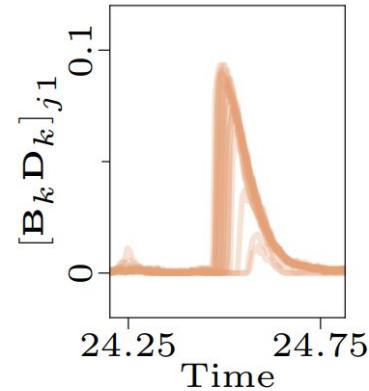
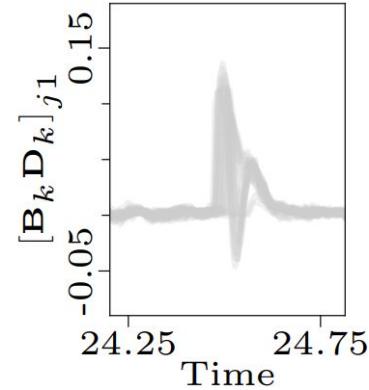
Constrained PARAFAC2 can improve interpretability in a chemometrics application



(a) ALS (non-negativity on \mathbf{A}_i and $\{\mathbf{D}_k\}_{k \leq K}$).



(b) AO-ADMM (non-negativity on all modes).



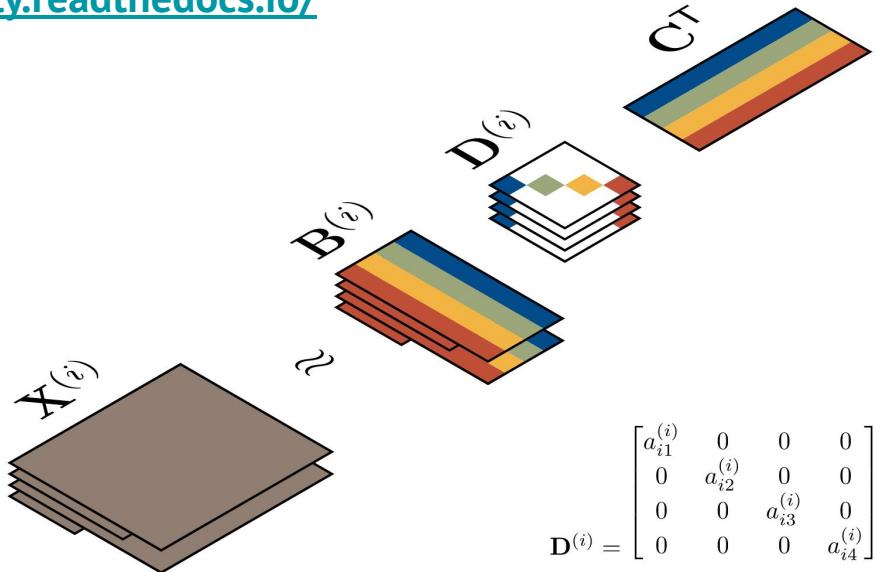
More details are available in our papers and on GitHub

- Roald M, Schenker C, Calhoun VD, Adalı T, Bro R, Cohen JE, Acar E. An AO-ADMM approach to constraining PARAFAC2 on all modes. Submitted to SIMODS, arXiv:2110.01278
 - Code at: GitHub.com/MarieRoald/PARAFAC2-AOADMM-SIMODS
- Roald M, Schenker C, Cohen JE, Acar E. PARAFAC2 AO-ADMM: Constraints in all modes. In 2021 29th European Signal Processing Conference (EUSIPCO) 2021 Aug 23 (pp. 1040-1044). IEEE.
 - Code at: GitHub.com/MarieRoald/PARAFAC2-AOADMM-EUSIPCO21

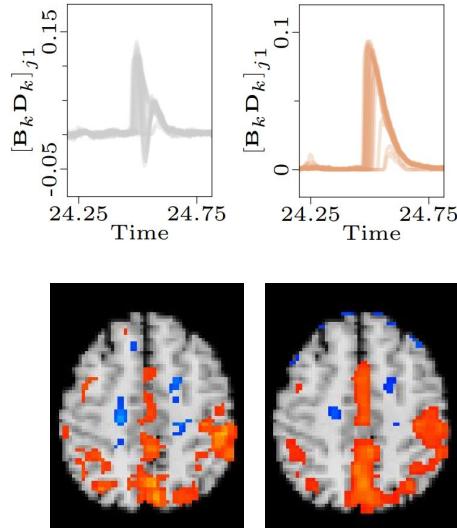
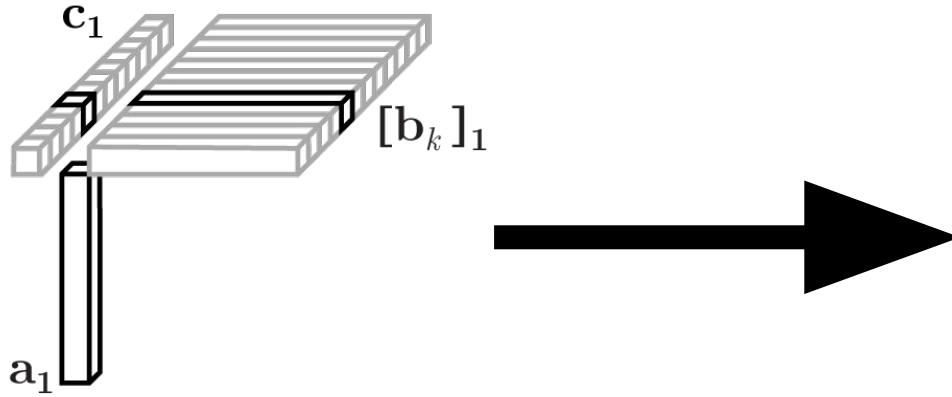
There is also a Python package for fitting constrained PARAFAC2 models with AO-ADMM

<https://github.com/MarieRoald/matcouply>

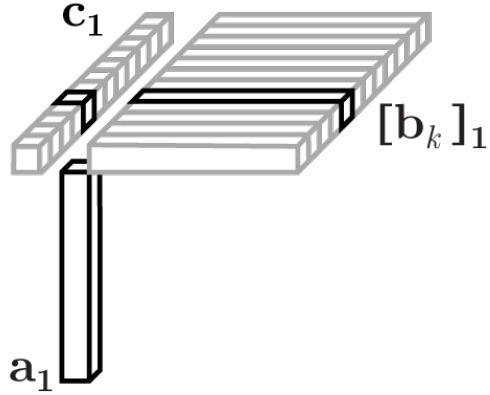
<https://matcouply.readthedocs.io/>



In summary, our AO-ADMM scheme allows for fitting PARAFAC2 with flexible constraints on all modes and such constraints can improve accuracy and interpretability



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Questions?

