Supplementary Material
PARAFAC2-based Coupled Matrix and Tensor Factorizations

Carla Schenker, Xiulin Wang, Evrim Acar

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1 ADMM for uncoupled modes of PARAFAC2

1.1 ADMM for $\mathbf{B}_k$

As first proposed in [1], the subproblem for the (regularized) varying mode $\mathbf{B}$ of the PARAFAC2 model,

$$\begin{aligned} \underset{\{\mathbf{B}_k\}_{k\leq K}}{\operatorname{argmin}} \quad & \sum_{k=1}^{K} w_1 \left\| \mathbf{X}_k - \mathbf{A}\mathbf{D}_k\mathbf{B}_k^T \right\|_F^2 + g_B(\mathbf{B}_k) \\ \text{s.t.} \quad & \{\mathbf{B}_k\}_{k\leq K} \in \mathcal{P} \end{aligned} \tag{5}$$

is solved using ADMM with the following splitting scheme:

$$\begin{aligned} \underset{\{\mathbf{B}_k\}_{k\leq K}}{\operatorname{argmin}} \quad & \sum_{k=1}^{K} w_1 \left\| \mathbf{X}_k - \mathbf{A}\mathbf{D}_k\mathbf{B}_k^T \right\|_F^2 + g_B(\mathbf{Z}_{B_k}) + \iota_{\mathcal{P}}(\mathbf{W}_{B_k}) \\ \text{s.t.} \quad & \mathbf{B}_k = \mathbf{Z}_{B_k}, \quad \forall k \leq K, \\ & \mathbf{B}_k = \mathbf{W}_{B_k}, \quad \forall k \leq K. \end{aligned} \tag{6}$$

This is in the standard form of problems that are solvable with ADMM, except the set $\mathcal{P}$, which describes the PARAFAC2 constraint, is not convex and the computation of the corresponding proximal operator is not straightforward. The ADMM algorithm is given in Algorithm 2.

Algorithm 2 ADMM for subproblem w.r.t. mode $\mathbf{B}$ of regularized PARAFAC2

while convergence criterion is not met **do**
  for $k = 1, ..., K$ **do**
$$\begin{aligned}\mathbf{B}_k^{(n+1)} &= \underset{\mathbf{B}_k}{\operatorname{argmin}}\ w_1 \left\| \mathbf{X}_k - \mathbf{A}\mathbf{D}_k\mathbf{B}_k^T \right\|_F^2 + \frac{\rho_{B_k}}{2}\left(\left\| \mathbf{B}_k - \mathbf{Z}_{B_k}^{(n)} + \boldsymbol{\mu}_{Z_{B_k}}^{(n)} \right\|_F^2 + \left\| \mathbf{B}_k - \mathbf{W}^{(n)} + \boldsymbol{\mu}_{\Delta_{B_k}}^{(n)} \right\|_F^2 \right) \\ &= \left[w_1 \mathbf{X}_k^T \mathbf{A}\mathbf{D}_k + \frac{\rho_{B_k}}{2}\left(\mathbf{Z}_{B_k}^{(n)} - \boldsymbol{\mu}_{Z_{B_k}}^{(n)} + \mathbf{W}^{(n)} - \boldsymbol{\mu}_{\Delta_{B_k}}^{(n)} \right) \right] \left[w_1 \mathbf{D}_k \mathbf{A}^T \mathbf{A}\mathbf{D}_k + \rho_{B_k}\mathbf{I} \right]^{-1}\end{aligned}$$
    $\mathbf{Z}_{B_k}^{(n+1)} = \operatorname{prox}_{\frac{1}{\rho_{B_k}} g_B}\left(\mathbf{B}_k^{(n+1)} + \boldsymbol{\mu}_{Z_{B_k}}^{(n)} \right)$
  end for
  $\left\{ \mathbf{W}_{B_k}^{(n+1)} \right\}_{k\leq K} = \operatorname{prox}_{\frac{1}{\rho_{B_k}} \iota_{\mathcal{P}}}\left(\left\{ \mathbf{B}_k^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_{B_k}}^{(n)} \right\}_{k\leq K} \right) \longleftarrow$ Algorithm 3
  for $k = 1, ..., K$ **do**
    $\boldsymbol{\mu}_{Z_{B_k}}^{(n+1)} = \boldsymbol{\mu}_{Z_{B_k}}^{(n)} + \mathbf{B}_k^{(n+1)} - \mathbf{Z}_{B_k}^{(n+1)}$
    $\boldsymbol{\mu}_{\Delta_{B_k}}^{(n+1)} = \boldsymbol{\mu}_{\Delta_{B_k}}^{(n)} + \mathbf{B}_k^{(n+1)} - \mathbf{W}_{B_k}^{(n+1)}$
  end for
  $n = n + 1$
end while

Note that both FOR-loops can be computed in parallel and a Cholesky decomposition of $\left[w_1 \mathbf{D}_k \mathbf{A}^T \mathbf{A} \mathbf{D}_k + \rho_{B_k} \mathbf{I}\right]$ is precomputed outside of the loop. For the evaluation of the proximal operator in line 6, we use the (standard) parametrization of the set $\mathcal{P}$, see [1], to obtain the following equivalent formulation:

$$\underset{\boldsymbol{\Delta}_B, \{\mathbf{P}_k\}_{k \leq K}}{\operatorname{argmin}} \left\| \left(\mathbf{B}_k + \boldsymbol{\mu}_{\Delta_{B_k}}\right) - \mathbf{P}_k \boldsymbol{\Delta}_B \right\|_F^2 + \iota_{orth}(\mathbf{P}_k). \tag{7}$$

In order to efficiently approximate this, we employ an AO scheme, where the orthogonal Procustes problem is solved independently for each $\mathbf{P}_k$, see Algorithm 3. We only use one iteration of Algorithm 3 for each ADMM iteration, as this is sufficient in our experience.

Algorithm 3 Approximate projection onto $\mathcal{P}$

while convergence criterion is not met **do**
    for $k = 1, ..., K$ **do**
        Compute SVD: $\mathbf{U}^{(k)} \boldsymbol{\Sigma}^{(k)} \mathbf{V}^{(k)^T} = \left(\mathbf{B}_k + \boldsymbol{\mu}_{\Delta_{B_k}}\right) \boldsymbol{\Delta}_B^T$
        $\mathbf{P}_k = \mathbf{U}^{(k)} \mathbf{V}^{(k)^T}$
    end for
    $\boldsymbol{\Delta}_B = \frac{1}{\sum_{k=1}^{K} \rho_{B_k}} \sum_{k=1}^{K} \rho_{B_k} \mathbf{P}_k^T \left(\mathbf{B}_k + \boldsymbol{\mu}_{\Delta_{B_k}}\right)$
end while

1.2 ADMM for C

The subproblem for regularized $\mathbf{C}$ ($\mathbf{D}_k = \operatorname{Diag}(\mathbf{C}_{k,:})$) with split variable $\mathbf{Z}_C$ ($\mathbf{Z}_{C_{k,:}} = \mathbf{z}_{C_k}$),

$$\begin{aligned} \underset{\mathbf{C}, \mathbf{Z}_C}{\operatorname{argmin}} \quad & \sum_{k=1}^{K} \left[w_1 \left\| \mathbf{X}_k - \mathbf{A} \operatorname{Diag}\left(\mathbf{C}_{k,:}\right) \mathbf{B}_k^T \right\|_F^2 + g_C(\mathbf{Z}_C) \right] \\ \text{s.t.} \quad & \mathbf{C} = \mathbf{Z}_C \end{aligned} \tag{8}$$

is vectorized as follows:

$$\begin{aligned} \underset{\mathbf{C}, \mathbf{Z}_C}{\operatorname{argmin}} \quad & \sum_{k=1}^{K} \left[w_1 \left\| \operatorname{vec}(\mathbf{X}_k) - (\mathbf{B}_k \odot \mathbf{A}) \mathbf{C}_{k,:}^T \right\|_2^2 + g_C(\mathbf{Z}_C) \right]. \\ \text{s.t.} \quad & \mathbf{C} = \mathbf{Z}_C \end{aligned} \tag{9}$$

Applying row-wise ADMM and the following transformations

$$\begin{aligned} (\mathbf{B}_k \odot \mathbf{A})^T (\mathbf{B}_k \odot \mathbf{A}) &= \mathbf{A}^T \mathbf{A} * \mathbf{B}_k^T \mathbf{B}_k, \\ (\mathbf{B}_k \odot \mathbf{A})^T \operatorname{vec}(\mathbf{X}_k) &= \operatorname{Diag}\left(\mathbf{A}^T \mathbf{X}_k \mathbf{B}_k\right), \end{aligned} \tag{10}$$

results in Algorithm 4, see also [1], where all rows k can be updated in parallel and a Cholesky decomposition of $\left[w_1 (\mathbf{A}^T \mathbf{A} * \mathbf{B}_k^T \mathbf{B}_k) + \frac{\rho_{C_k}}{2} \mathbf{I}_R\right]$ is precomputed.

Algorithm 4 ADMM for subproblem w.r.t. mode $\mathbf{C}$ of regularized PARAFAC2

while convergence criterion is not met **do**
  for $k = 1, ..., K$ **do**
    $$\mathbf{C}_{k,:}^{(n+1)^T} = \underset{\mathbf{c}}{\operatorname{argmin}}\ w_1 \parallel \operatorname{vec}(\mathbf{X}_k) - (\mathbf{B}_k \odot \mathbf{A})\mathbf{c} \parallel_2^2 + \frac{\rho_{C_k}}{2} \left\| \mathbf{c} - \mathbf{z}_{C_k}^{(n)} + \boldsymbol{\mu}_{z_{C_k}}^{(n)} \right\|_2^2$$
    $$= \left[w_1(\mathbf{A}^T\mathbf{A} * \mathbf{B}_k^T\mathbf{B}_k) + \frac{\rho_{C_k}}{2}\mathbf{I}_R \right]^{-1} \left[w_1 \operatorname{Diag}\left(\mathbf{A}^T\mathbf{X}_k\mathbf{B}_k\right) + \frac{\rho_{C_k}}{2}\left(\mathbf{z}_{C_k}^{(n)} - \boldsymbol{\mu}_{z_{C_k}}^{(n)}\right)\right]$$
  end for
  $\mathbf{Z}_C^{(n+1)} = \operatorname{prox}_{\frac{1}{\max \rho_{C_k}} g_C}\left(\mathbf{C}^{(n+1)} + \boldsymbol{\mu}_{Z_C}^{(n)}\right)$
  $\boldsymbol{\mu}_{Z_C}^{(n+1)} = \boldsymbol{\mu}_{Z_C}^{(n)} + \mathbf{C}^{(n+1)} - \mathbf{Z}_C^{(n+1)}$
  $n = n + 1$
end while

2 ADMM for F

The regularized, but uncoupled mode of the matrix decomposition $\mathbf{F}$ is updated using standard ADMM, see also [2], as follows:

Algorithm 5 ADMM for subproblem w.r.t. $\mathbf{F}$

while convergence criterion is not met **do**
  $\mathbf{F}^{(n+1)} = \left[w_2\mathbf{Y}^T\mathbf{E} + \frac{\rho_F}{2}\left(\mathbf{Z}_F^{(n)} - \boldsymbol{\mu}_{Z_F}^{(n)}\right)\right] \left[w_2\mathbf{E}^T\mathbf{E} + \frac{\rho_A}{2}\mathbf{I}_{R_2}\right]^{-1}$
  $\mathbf{Z}_F^{(n+1)} = \operatorname{prox}_{\frac{1}{\rho_F} g_F}\left(\mathbf{F}^{(n+1)} + \boldsymbol{\mu}_{Z_F}^{(n)}\right)$
  $\boldsymbol{\mu}_{Z_F}^{(n+1)} = \boldsymbol{\mu}_{Z_F}^{(n)} + \mathbf{F}^{(n+1)} - \mathbf{Z}_F^{(n+1)}$
  $n = n + 1$
end while

3 Update for coupled modes for different linear couplings

For the four different types of linear couplings described in [2], the updates of $\mathbf{A}, \mathbf{E}, \boldsymbol{\Delta}, \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}$ and $\boldsymbol{\mu}_{\boldsymbol{\Delta}_E}$ in Algorithm 1 have to be adapted. We give the specific updates for each case in the following. For restrictions on the transformation matrices $\tilde{\mathbf{H}}_{\mathbf{A}}, \tilde{\mathbf{H}}_{\mathbf{E}}, \tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}, \tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}$,..., we refer to the supplementary material of [2].

3.1 Case $2a$

Linear couplings of type:

$$\tilde{\mathbf{H}}_{\mathbf{A}}\mathbf{A} = \boldsymbol{\Delta}, \quad \tilde{\mathbf{H}}_{\mathbf{E}}\mathbf{E} = \boldsymbol{\Delta} \tag{11}$$

For the update of $\mathbf{A}$, the following Sylvester equation has to be solved:

$$\begin{aligned} &\frac{\rho_A}{2}\left(\mathbf{I}_{R_1} + \tilde{\mathbf{H}}_{\mathbf{A}}^T\tilde{\mathbf{H}}_{\mathbf{A}}\right)\mathbf{A}^{(n+1)} + \mathbf{A}^{(n+1)} w_1 \sum_{k=1}^{K} \mathbf{D}_k\mathbf{B}_k^T\mathbf{B}_k\mathbf{D}_k = \\ &\qquad w_1 \sum_{k=1}^{K} \mathbf{X}_k\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\left[\mathbf{Z}_A^{(n)} - \boldsymbol{\mu}_{Z_A}^{(n)} + \tilde{\mathbf{H}}_{\mathbf{A}}^T\left(\boldsymbol{\Delta}^{(n)} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right)\right] \end{aligned} \tag{12}$$

For the update of $\mathbf{E}$, the following Sylvester equation has to be solved:

$$\frac{\rho_E}{2}\left(\mathbf{I}_{R_2} + \tilde{\mathbf{H}}_{\mathbf{E}}^T\tilde{\mathbf{H}}_{\mathbf{E}}\right)\mathbf{E}^{(n+1)} + \mathbf{E}^{(n+1)} w_2\mathbf{F}^T\mathbf{F} = w_2\mathbf{Y}\mathbf{E} + \frac{\rho_E}{2}\left[\mathbf{Z}_E^{(n)} - \boldsymbol{\mu}_{Z_E}^{(n)} + \tilde{\mathbf{H}}_{\mathbf{E}}^T\left(\boldsymbol{\Delta}^{(n)} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\right] \tag{13}$$

The update of $\boldsymbol{\Delta}$ is given by an average:

$$\boldsymbol{\Delta}^{(n+1)} = \frac{1}{\rho_A+\rho_E}\left[\rho_A\left(\tilde{\mathbf{H}}_{\mathbf{A}}\mathbf{A}^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right) + \rho_E\left(\tilde{\mathbf{H}}_{\mathbf{E}}\mathbf{E}^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\right] \tag{14}$$

And finally,

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)} + \tilde{\mathbf{H}}_{\mathbf{A}}\mathbf{A}^{(n+1)} - \boldsymbol{\Delta}^{(n+1)}, \tag{15}$$

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)} + \tilde{\mathbf{H}}_{\mathbf{E}}\mathbf{E}^{(n+1)} - \boldsymbol{\Delta}^{(n+1)}. \tag{16}$$

3.2 Case $2b$

Linear couplings of type:

$$\mathbf{A} = \tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}\boldsymbol{\Delta}, \quad \mathbf{E} = \tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}\boldsymbol{\Delta} \tag{17}$$

For the update of $\mathbf{A}$, the following linear system has to be solved:

$$\mathbf{A}^{(n+1)}\left[w_1\sum_{k=1}^{K}\mathbf{D}_k\mathbf{B}_k^T\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\ (\mathbf{I}_{R_1} + \mathbf{I}_{R_1})\right] = \left[w_1\sum_{k=1}^{K}\mathbf{X}_k\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\left(\mathbf{Z}_A^{(n)} - \boldsymbol{\mu}_{Z_A}^{(n)} + \tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}\boldsymbol{\Delta}^{(n)} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right)\right] \tag{18}$$

For the update of $\mathbf{E}$, the following linear system has to be solved:

$$\mathbf{E}^{(n+1)}\left[w_2\mathbf{F}^T\mathbf{F} + \frac{\rho_E}{2}\left(\mathbf{I}_{R_2} + \mathbf{I}_{R_2}\right)\right] = \left[w_2\mathbf{Y}\mathbf{F} + \frac{\rho_E}{2}\left(\mathbf{Z}_E^{(n)} - \boldsymbol{\mu}_{Z_E}^{(n)} + \tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}\boldsymbol{\Delta}^{(n)} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\right] \tag{19}$$

For the update of $\boldsymbol{\Delta}$, the following linear system has to be solved:

$$\left(\rho_A\tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}\,T}\tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}} + \rho_E\tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}\,T}\tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}\right)\boldsymbol{\Delta}^{(n+1)} = \rho_A\tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}\,T}\left(\mathbf{A}^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right) + \rho_E\tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}\,T}\left(\mathbf{E}^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right) \tag{20}$$

And finally,

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)} + \mathbf{A}^{(n+1)} - \tilde{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}\boldsymbol{\Delta}^{(n+1)}, \tag{21}$$

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)} + \mathbf{E}^{(n+1)} - \tilde{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}\boldsymbol{\Delta}^{(n+1)}. \tag{22}$$

3.3 Case $3a$

Linear couplings of type:

$$\mathbf{A}\hat{\mathbf{H}}_{\mathbf{A}} = \boldsymbol{\Delta}, \quad \mathbf{E}\hat{\mathbf{H}}_{\mathbf{E}} = \boldsymbol{\Delta} \tag{23}$$

For the update of $\mathbf{A}$, the following linear system has to be solved:

$$\mathbf{A}^{(n+1)}\left[w_1\sum_{k=1}^{K}\mathbf{D}_k\mathbf{B}_k^T\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\left(\mathbf{I}_{R_1} + \hat{\mathbf{H}}_{\mathbf{A}}\hat{\mathbf{H}}_{\mathbf{A}}^T\right)\right] = \left[w_1\sum_{k=1}^{K}\mathbf{X}_k\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\left(\mathbf{Z}_A^{(n)} - \boldsymbol{\mu}_{Z_A}^{(n)} + \left(\boldsymbol{\Delta}^{(n)} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right)\hat{\mathbf{H}}_{\mathbf{A}}^T\right)\right] \tag{24}$$

For the update of $\mathbf{E}$, the following linear system has to be solved:

$$\mathbf{E}^{(n+1)}\left[w_2\mathbf{F}^T\mathbf{F} + \frac{\rho_E}{2}\left(\mathbf{I}_{R_1} + \hat{\mathbf{H}}_{\mathbf{E}}\hat{\mathbf{H}}_{\mathbf{E}}^T\right)\right] = \left[w_2\mathbf{Y}\mathbf{F} + \frac{\rho_E}{2}\left(\mathbf{Z}_E^{(n)} - \boldsymbol{\mu}_{Z_E}^{(n)} + \left(\boldsymbol{\Delta}^{(n)} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\hat{\mathbf{H}}_{\mathbf{E}}^T\right)\right] \tag{25}$$

The update of $\boldsymbol{\Delta}$ is given by an average:

$$\boldsymbol{\Delta}^{(n+1)} = \tfrac{1}{\rho_A+\rho_E}\left[\rho_A\left(\mathbf{A}^{(n+1)}\hat{\mathbf{H}}_{\mathbf{A}} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right) + \rho_E\left(\mathbf{E}^{(n+1)}\hat{\mathbf{H}}_{\mathbf{E}} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\right] \tag{26}$$

And finally,

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)} + \mathbf{A}^{(n+1)}\hat{\mathbf{H}}_{\mathbf{A}} - \boldsymbol{\Delta}^{(n+1)}, \tag{27}$$

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)} + \mathbf{E}^{(n+1)}\hat{\mathbf{H}}_{\mathbf{E}} - \boldsymbol{\Delta}^{(n+1)}. \tag{28}$$

3.4 Case $3b$

Linear couplings of type:

$$\mathbf{A} = \boldsymbol{\Delta}\hat{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}, \quad \mathbf{E} = \boldsymbol{\Delta}\hat{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}} \tag{29}$$

For the update of $\mathbf{A}$, the following linear system has to be solved:

$$\begin{aligned}\mathbf{A}^{(n+1)}&\left[w_1\sum_{k=1}^{K}\mathbf{D}_k\mathbf{B}_k^T\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\ (\mathbf{I}_{R_1}+\mathbf{I}_{R_1})\right] = \\ &\left[w_1\sum_{k=1}^{K}\mathbf{X}_k\mathbf{B}_k\mathbf{D}_k + \frac{\rho_A}{2}\left(\mathbf{Z}_A^{(n)} - \boldsymbol{\mu}_{Z_A}^{(n)} + \boldsymbol{\Delta}^{(n)}\hat{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right)\right]\end{aligned} \tag{30}$$

For the update of $\mathbf{E}$, the following linear system has to be solved:

$$\mathbf{E}^{(n+1)}\left[w_2\mathbf{F}^T\mathbf{F} + \frac{\rho_E}{2}\left(\mathbf{I}_{R_2}+\mathbf{I}_{R_2}\right)\right] = \left[w_2\mathbf{Y}\mathbf{F} + \frac{\rho_E}{2}\left(\mathbf{Z}_E^{(n)} - \boldsymbol{\mu}_{Z_E}^{(n)} + \boldsymbol{\Delta}^{(n)}\hat{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}} - \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\right] \tag{31}$$

For the update of $\boldsymbol{\Delta}$, the following linear system has to be solved:

$$\boldsymbol{\Delta}^{(n+1)}\left(\rho_A\hat{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}\hat{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}^T} + \rho_E\hat{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}\hat{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}^T}\right) = \rho_A\left(\mathbf{A}^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)}\right)\hat{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}^T} + \rho_E\left(\mathbf{E}^{(n+1)} + \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)}\right)\hat{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}^T} \tag{32}$$

And finally,

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_A}^{(n)} + \mathbf{A}^{(n+1)} - \boldsymbol{\Delta}^{(n+1)}\hat{\mathbf{H}}_{\mathbf{A}}^{\boldsymbol{\Delta}}, \tag{33}$$

$$\boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n+1)} = \boldsymbol{\mu}_{\boldsymbol{\Delta}_E}^{(n)} + \mathbf{E}^{(n+1)} - \boldsymbol{\Delta}^{(n+1)}\hat{\mathbf{H}}_{\mathbf{E}}^{\boldsymbol{\Delta}}. \tag{34}$$

4 Stopping conditions

4.1 Inner ADMM loops

4.1.1 The varying mode $\mathbf{B}_k$ of PARAFAC2

The ADMM loop for $\mathbf{B}_k$ is stopped when a maximum number of iterations is reached, here 5, or when all of the following conditions are satisfied, (similar to [1]),

$$\begin{aligned}&\frac{1}{K}\sum_k\left(\|\mathbf{B}_k^{(n)} - \mathbf{Z}_{B_k}^{(n)}\|_F/\|\mathbf{B}_k^{(n)}\|_F\right) \le \epsilon^{\mathrm{p,constr}}\\ &\frac{1}{K}\sum_k\left(\|\mathbf{B}_k^{(n)} - \mathbf{P}_k^{(n)}\boldsymbol{\Delta}_B^{(n)}\|_F/\|\mathbf{B}_k^{(n)}\|_F\right) \le \epsilon^{\mathrm{p,coupl}}\\ &\frac{1}{K}\sum_k\left(\|\mathbf{Z}_{B_k}^{(n+1)} - \mathbf{Z}_{B_k}^{(n)}\|_F/\|\boldsymbol{\mu}_{Z_{B_k}}^{(n)}\|_F\right) \le \epsilon^{\mathrm{d,constr}}\\ &\frac{1}{K}\sum_k\left(\|\mathbf{P}_k^{(n+1)}\boldsymbol{\Delta}_B^{(n+1)} - \mathbf{P}_k^{(n)}\boldsymbol{\Delta}_B^{(n)}\|_F/\|\boldsymbol{\mu}_{\Delta_{B_k}}^{(n)}\|_F\right) \le \epsilon^{\mathrm{d,coupl}}\end{aligned} \tag{35}$$

where we set all tolerances to 10^{-5}.

4.1.2 Other modes

The other ADMM loops are stopped when a maximum number of iterations is reached, here 5, or when all of the following conditions are satisfied, (here given for the coupled modes $\mathbf{A}$ and $\mathbf{E}$, but equivalently for uncoupled but constrained modes, same as in [2]),

$$
\begin{aligned}
&\frac{1}{2}\left(\|\mathbf{E}^{(n)}-\mathbf{Z}_E^{(n)}\|_F/\|\mathbf{E}^{(n)}\|_F+\|\mathbf{A}^{(n)}-\mathbf{Z}_A^{(n)}\|_F/\|\mathbf{A}^{(n)}\|_F\right)\leq\epsilon^{\mathrm{p,constr}}\\
&\frac{1}{2}\left(\|\mathbf{H}_E\operatorname{vec}(\mathbf{E}^{(n)})-\mathbf{H}_E^{\Delta}\operatorname{vec}(\mathbf{\Delta}^{(n)})\|_2/\|\mathbf{H}_E\operatorname{vec}(\mathbf{E}^{(n)})\|_2\right.\\
&\qquad\qquad\qquad\left.+\|\mathbf{H}_A\operatorname{vec}(\mathbf{A}^{(n)})-\mathbf{H}_A^{\Delta}\operatorname{vec}(\mathbf{\Delta}^{(n)})\|_2/\|\mathbf{H}_A\operatorname{vec}(\mathbf{A}^{(n)})\|_2\right)\leq\epsilon^{\mathrm{p,coupl}}\\
&\frac{1}{2}\left(\|\mathbf{Z}_E^{(n+1)}-\mathbf{Z}_E^{(n)}\|_F/\|\boldsymbol{\mu}_{Z_E}^{(n)}\|_F+\|\mathbf{Z}_A^{(n+1)}-\mathbf{Z}_A^{(n)}\|_F/\|\boldsymbol{\mu}_{Z_A}^{(n)}\|_F\right)\leq\epsilon^{\mathrm{d,constr}}\\
&\frac{1}{2}\left(\|\mathbf{H}_E^{\Delta}\left(\operatorname{vec}(\mathbf{\Delta}^{(n+1)})-\operatorname{vec}(\mathbf{\Delta}^{(n)})\right)\|_2/\|\boldsymbol{\mu}_{\mathbf{\Delta}_E}^{(n)}\|_2\right.\\
&\qquad\qquad\qquad\left.+\|\mathbf{H}_A^{\Delta}\left(\operatorname{vec}(\mathbf{\Delta}^{(n+1)})-\operatorname{vec}(\mathbf{\Delta}^{(n)})\right)\|_2/\|\boldsymbol{\mu}_{\mathbf{\Delta}_A}^{(n)}\|_2\right)\leq\epsilon^{\mathrm{d,coupl}}
\end{aligned}
\tag{36}
$$

where we set all tolerances to 10^{-5}.

4.2 Outer AO loop

The whole algorithm is terminated, when each of the following residuals $f_\star^{(n)}$,

$$
\begin{aligned}
f_{\text{tensors}}^{(n)}=&w_1\sum_{k=1}^{K}\|\mathbf{X}_k-\mathbf{A}\mathbf{D}_k\mathbf{B}_k^T\|_F^2+w_2\|\mathbf{Y}-\mathbf{E}\mathbf{F}^T\|_F^2\\
f_{\text{couplings}}^{(n)}=&\frac{1}{2}\left(\|\mathbf{H}_A\operatorname{vec}(\mathbf{A}^{(n)})-\mathbf{H}_A^{\Delta}\operatorname{vec}(\mathbf{\Delta}^{(n)})\|_2/\|\mathbf{H}_A\operatorname{vec}(\mathbf{A}^{(n)})\|_2\right.\\
&\left.+\|\mathbf{H}_E\operatorname{vec}(\mathbf{E}^{(n)})-\mathbf{H}_E^{\Delta}\operatorname{vec}(\mathbf{\Delta}^{(n)})\|_2/\|\mathbf{H}_E\operatorname{vec}(\mathbf{E}^{(n)})\|_2\right)\\
f_{\text{PAR2constraint}}^{(n)}=&\frac{1}{K}\sum_{k=1}^{K}\left(\|\mathbf{B}_k^{(n)}-\mathbf{P}_k^{(n)}\mathbf{\Delta}_B^{(n)}\|_F/\|\mathbf{B}_k^{(n)}\|_F\right)\\
f_{\text{constraints}}^{(n)}=&\frac{1}{5}\left(\|\mathbf{A}^{(n)}-\mathbf{Z}_A^{(n)}\|_F/\|\mathbf{A}^{(n)}\|_F+\|\mathbf{C}^{(n)}-\mathbf{Z}_C^{(n)}\|_F/\|\mathbf{C}^{(n)}\|_F\right.\\
&+\frac{1}{K}\sum_{k=1}^{K}\left(\|\mathbf{B}_k^{(n)}-\mathbf{Z}_{B_k}^{(n)}\|_F/\|\mathbf{B}_k^{(n)}\|_F\right)\\
&\left.+\|\mathbf{E}^{(n)}-\mathbf{Z}_E^{(n)}\|_F/\|\mathbf{E}^{(n)}\|_F+\|\mathbf{F}^{(n)}-\mathbf{Z}_F^{(n)}\|_F/\|\mathbf{F}^{(n)}\|_F\right)
\end{aligned}
\tag{37}
$$

has either reached a small absolute tolerance $\epsilon^{\mathrm{abs,outer}}$, or has not changed more than some small relative tolerance $\epsilon^{\mathrm{rel,outer}}$ compared to the previous iteration,

$$
f_\star^{(n)}<\epsilon^{\mathrm{abs,outer}},\qquad|f_\star^{(n)}-f_\star^{(n-1)}|/|f_\star^{(n)}|<\epsilon^{\mathrm{rel,outer}}
$$

or a predefined number of maximal outer iterations is reached. Here, we set the maximum number of outer iterations to 4000 and the outer absolute and relative tolerances to be 10^{-7} and 10^{-8}, respectively.

5 Efficient computation of the PARAFAC2 residual

As described in [2] for the residual in CP decomposition, also the PARAFAC2 residual can be computed efficiently, via the equivalent formulation

$$
\sum_{k=1}^{K}\|\mathbf{X}_k-\mathbf{M}_k\|_F^2=\sum_{k=1}^{K}\|\mathbf{X}_k\|_F^2+\sum_{k=1}^{K}\|\mathbf{M}_k\|_F^2-2\sum_{k=1}^{K}\langle\mathbf{X}_k,\mathbf{M}_k\rangle\,,
\tag{38}
$$

where $\mathbf{M}_k = \mathbf{A}\mathbf{D}_k\mathbf{B}_k^T$. The term $\sum_{k=1}^{K} \| \mathbf{X}_k \|_F^2$ is constant and can be precomputed. Furthermore, it holds

$$\sum_{k=1}^{K} \| \mathbf{M}_k \|_F^2 = \sum_{k=1}^{K} \mathbf{e}^T \left[\mathbf{A}^T\mathbf{A} * (\mathbf{B}_k\mathbf{D}_k)^T(\mathbf{B}_k\mathbf{D}_k) \right] \mathbf{e} = \mathbf{e}^T \left[\mathbf{A}^T\mathbf{A} * \sum_{k=1}^{K} \mathbf{D}_k\mathbf{B}_k^T\mathbf{B}_k\mathbf{D}_k \right] \mathbf{e}, \tag{39}$$

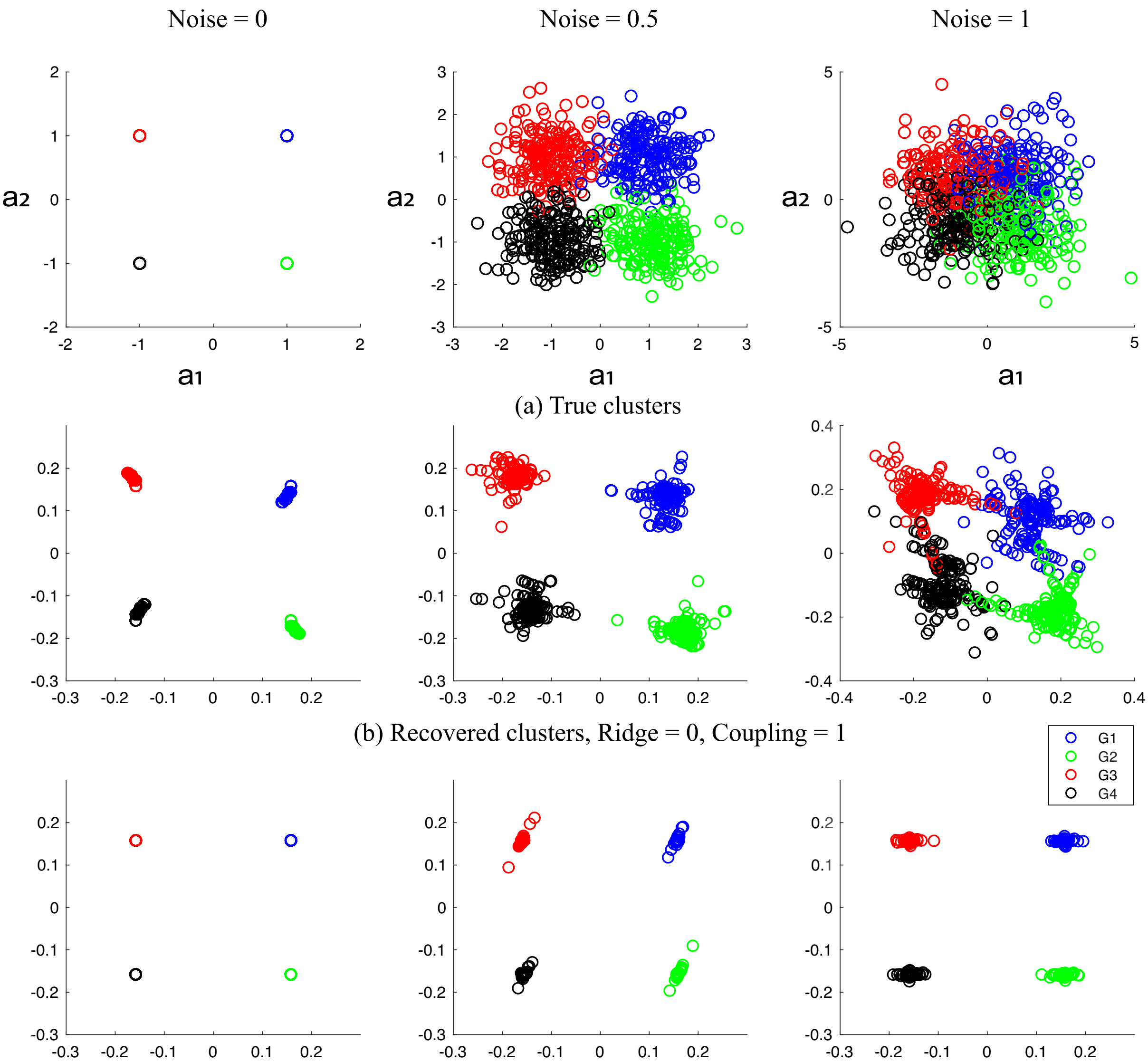
where $\mathbf{e}$ is a vector of all ones of matching length. When the mode $\mathbf{A}$ is updated last (after $\mathbf{B}_k$ and $\mathbf{D}_k$), then the term $\sum_{k=1}^{K} \mathbf{D}_k\mathbf{B}_k^T\mathbf{B}_k\mathbf{D}_k$ has already been computed in the update of $\mathbf{A}$ and can be used for residual computation. The same holds for the term

$$\sum_{k=1}^{K} \langle \mathbf{X}_k, \mathbf{M}_k \rangle = \mathbf{e}^T \left[\sum_{k=1}^{K} \mathbf{X}_k\mathbf{B}_k\mathbf{D}_k * \mathbf{A} \right] \mathbf{e}, \tag{40}$$

where $\sum_{k=1}^{K} \mathbf{X}_k\mathbf{B}_k\mathbf{D}_k$ is already computed in the last update of $\mathbf{A}$.

6 Details on Experiments

6.1 Experiment 2



(a) True clusters

(b) Recovered clusters, Ridge = 0, Coupling = 1

(c) Recovered clusters, Ridge = 1e-4, Coupling = 1

Figure 7: Exp. 2: Illustration of clustering structures from 20 different runs when noise = 0, 0.5 and 1 in (a) the ground-truth $\mathbf{A}$, (b) recovered $\mathbf{A}$ using exact coupling and no ridge regularization, (c) recovered $\mathbf{A}$ using exact coupling and ridge regularization where the penalty parameter is set to $1e-4$.

6.2 Experiment 3

Table 3: Average model fit and FMS values for experiment 3.

Fit (%)		FMS					
PAR2	CP	A	B	C	E	F	G
96.16	96.19	1	0.99	1	1	1	1

References

[1] M. Roald, C. Schenker, V. D. Calhoun, T. Adali, R. Bro, J. E. Cohen, and E. Acar, "An AO-ADMM approach to constraining PARAFAC2 on all modes," *SIAM Journal on Mathematics of Data Science*, vol. 4, no. 3, pp. 1191–1222, 2022.

[2] C. Schenker, J. E. Cohen, and E. Acar, "A flexible optimization framework for regularized matrix-tensor factorizations with linear couplings," *IEEE Journal of Selected Topics in Signal Processing*, vol. 15, no. 3, pp. 506–521, 2020.