Supplements for “Multi-way block localization via sparse tensor clustering”

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A Proofs

A.1 Proof of Proposition 1

Let $\mathcal{S} = \{\mathbb{P}_\Theta \colon \Theta \in \mathcal{P}\}$ be the family of (either Gaussian or Bernoulli) tensor block models (2), where $\Theta = \mathcal{C} \times_1 \boldsymbol{M}_1 \times_2 \cdots \times_K \boldsymbol{M}_K$ parameterizes the mean block tensor. Since the mapping $\Theta \mapsto \mathbb{P}_\Theta$ is one-to-one, Θ is identifiable. Now suppose there are two decompositions of $\Theta = \Theta(\{\boldsymbol{M}_k\}, \mathcal{C}) = \Theta(\{\tilde{\boldsymbol{M}}_k\}, \tilde{\mathcal{C}})$. Based on the Assumption 1, we have

$$\Theta = \mathcal{C} \times_1 \boldsymbol{M}_1 \times_2 \cdots \times_K \boldsymbol{M}_K = \tilde{\mathcal{C}} \times_1 \tilde{\boldsymbol{M}}_1 \times_2 \cdots \times_K \tilde{\boldsymbol{M}}_K, \tag{1}$$

where $\mathcal{C}, \tilde{\mathcal{C}} \in \mathbb{R}^{R_1 \times \cdots \times R_K}$ are two irreducible cores, and $\boldsymbol{M}_k, \tilde{\boldsymbol{M}}_k \in \{0,1\}^{R_k \times d_k}$ are membership matrices for all $k \in [K]$. We will prove by contradiction that $\boldsymbol{M}_k$ and $\tilde{\boldsymbol{M}}_k$ induce the same partition of $[d_k]$, for all $k \in [K]$.

Suppose the above claim does not hold. Then there exists a mode $k \in [K]$ such that the $\boldsymbol{M}_k, \tilde{\boldsymbol{M}}_k$ induce two different partitions of $[d_k]$. Without loss of generality, we assume $k = 1$. The definition of partition implies that there exists a pair of indices $i \neq j, i, j \in [d_1]$, such that, i, j belong to the same cluster based on $\boldsymbol{M}_k$, but they belong to different clusters based on $\tilde{\boldsymbol{M}}_k$. Let $\mathcal{C} \subset [d_1]$ denote the cluster that i (or j) belong to based on $\boldsymbol{M}_k$, and $\mathcal{A}, \mathcal{B} \subset [d_1]$ denote the two different clusters that i, j belongs to based on $\tilde{\boldsymbol{M}}_k$. Based on the left-hand side of (1)

$$\Theta_{i,i_2,\ldots,i_K} = \Theta_{j,i_2,\ldots,i_K}, \quad \text{for all } (i_2, \ldots, i_K) \in [d_2] \times \cdots \times [d_K]. \tag{2}$$

On the other hand, (1) implies

$$\Theta_{i,i_2,\ldots,i_K} = \Theta_{k,i_2,\ldots,i_K}, \quad \text{for all } k \in \mathcal{A} \text{ and } (i_2, \ldots, i_K) \in [d_2] \times \cdots \times [d_K], \tag{3}$$

and

$$\Theta_{j,i_2,\ldots,i_K} = \Theta_{k,i_2,\ldots,i_K}, \quad \text{for all } k \in \mathcal{B} \text{ and } (i_2, \ldots, i_K) \in [d_2] \times \cdots \times [d_K]. \tag{4}$$

Combining (2), (3) and (4), we have

$$\Theta i, i_2, \ldots, i_K = \Theta_{k,i_2,\ldots,i_K}, \quad \text{for all } k \in \mathcal{A} \cup \mathcal{B} \text{ and } (i_2, \ldots, i_K) \in [d_2] \times \cdots \times [d_K].$$

Therefore, one can merge $\mathcal{A}, \mathcal{B}$ into one cluster along the mode 1. This contradicts the irreducibility of the core tensor $\tilde{\mathcal{C}}$. Therefore, $\boldsymbol{M}_1$ and $\tilde{\boldsymbol{M}}_1$ induce a same partition of $[d_1]$, and thus they are equal up to permutations. The proof is now complete.

A.2 Proof of Theorem 1

To study the performance of the least-square estimator $\hat{\Theta}$, we need to introduce some additional notations. We view the membership matrix $\boldsymbol{M}_k$ as a onto function $\boldsymbol{M}_k \colon [d_k] \mapsto [R_k]$, and with a little abuse of notation, we still use $\boldsymbol{M}_k$ to denote the mapping function. Correspondingly, we use

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$\boldsymbol{M}_k(i) \in [R_k]$ to denote the cluster label for the element $i \in [d_k]$. The parameter space $\mathcal{P}$ can be equivalently written as

$$\begin{aligned}\mathcal{P} =& \big\{\Theta \in \mathbb{R}^{d_1\times\cdots\times d_K} \colon \Theta_{i_1,\ldots,i_K} = \mathcal{C}_{r_1,\ldots,r_K} \text{ for } (i_1,\ldots,i_K) \in \boldsymbol{M}_1^{-1}(r_1)\times\cdots\times\boldsymbol{M}_K^{-1}(r_K)\\ &\quad \text{with some membership matrices } \boldsymbol{M}_k\text{'s and a core tensor } \mathcal{C}\in\mathbb{R}^{R_1\times\cdots\times R_K}\big\}.\end{aligned}$$

In other words, the mean signal tensor Θ is a piecewise constant with respect to the blocks in the Cartesian product of the mode-k clusters, $\boldsymbol{M}_1^{-1}(r_1)\times\cdots\times\boldsymbol{M}_K^{-1}(r_K)$, for all $(r_1,\ldots,r_K) \in [R_1]\times\cdots\times[R_K]$.

Let $d = \prod_k d_k$ and $R = \prod_k R_k$. We define $\mathcal{D}(s)$ to be the set of d-dimensional vectors with at most s distinct entry values. By identifying the tensors in $\mathcal{P}$ as d-dimensional vectors, we have $\mathcal{P} \subset \mathcal{D}^d(R)$.

Now consider the least-estimate estimator

$$\hat{\Theta} = \arg\min_{\Theta\in\mathcal{P}}\{-2\langle\mathcal{Y},\Theta\rangle + \|\Theta\|_F^2\} = \arg\min_{\Theta\in\mathcal{P}}\{\|\mathcal{Y}-\Theta\|_F^2\}.$$

Based on Proposition **??**, we have

$$\|\hat{\Theta}-\Theta_{\text{true}}\|_F \le 2\sup_{\mu\in(\mathcal{P}-\mathcal{P}')\cap\boldsymbol{B}_2^d}\langle\mu,\mathcal{E}\rangle,$$

where $(\mathcal{P}-\mathcal{P}') = \{\mu-\mu' \colon \mu,\mu'\in\mathcal{P}\}$ and $\boldsymbol{B}_2^d$ denotes the Euclidean unit ball in dimension d. Based on the definition we have

$$(\mathcal{P}-\mathcal{P}') \subset \mathcal{D}^d(R^2).$$

(to be finished...)

$$\begin{aligned}\sup_{\mu\in(\mathcal{P}-\mathcal{P}')\cap\boldsymbol{B}_2^d}\langle\mu,\mathcal{E}\rangle &\le \sup_{\mu\in\mathcal{D}(R^2)\cap\boldsymbol{B}_2^d}\langle\mu,\mathcal{E}\rangle && (5)\\ &\le \sup_{|\boldsymbol{s}|=R^2}\sup_{\mu\in\boldsymbol{B}_2^{\boldsymbol{s}}}\langle\mu,\mathcal{E}\rangle && (6)\\ &\le 2\sigma\log\left(6^{R^2}\binom{d}{R^2}\right) && (7)\\ &\le 2\sigma R^2 + ... && (8)\end{aligned}$$

with probability at least $1-\exp(R^2)$

For fixed $\boldsymbol{M}_k$'s, $\mathcal{C}$ is a linear space of dimension no greater than R^2.

A.3 Proof of

A.4 Sparse clustering

Lemma 1

Let $\mathbf{Y}\in\mathbb{R}^n$ be a response vector and $\mathbf{X}\in\mathbb{R}^{n\times p}$ the design matrix. Assume the response vector $\mathbf{Y}$ is mean-centered, i.e., $\sum_i Y_i = 0$. Suppose that $\mathbf{X}$ is an orthogonal design matrix with $X^TX = diag(n_1,...,n_p)$. Define the ordinary least-square estimate $\hat{\boldsymbol{\beta}}_{ols} = (\hat{\beta}_{ols,1},...,\hat{\beta}_{ols,p}^T)^T$. Consider the following constrained optimization:

$$\hat{\boldsymbol{\beta}} = \arg\min\{\frac{1}{2}||\mathbf{Y}-\mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda pen(\boldsymbol{\beta})\}$$

1. Case 1: L-0 penalization. $pen(\boldsymbol{\beta}) = ||\boldsymbol{\beta}||_0$:
Under the change of tuning parameter $\lambda' := f(\lambda) = \sqrt{2\lambda}$ such that $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1,...,\hat{\beta}_p)^T$ has a closed-form solution:

$$\hat{\beta}_i = \hat{\beta}_{ols,i}\mathbb{I}_{|\hat{\beta}_{ols,i}|>\frac{\lambda'}{\sqrt{n_i}}}\ for\ all\ i=1,...,p$$

2. Case 2: L-1 penalization. $pen(\boldsymbol{\beta}) = ||\boldsymbol{\beta}||_1$:
$\hat{\boldsymbol{\beta}} = (\hat{\beta}_1,...,\hat{\beta}_p)^T$ has a closed-form solution:

$$\hat{\beta}_i = sign(\hat{\beta_{ols,i}})(|\hat{\beta_{ols,i}}| - \frac{\lambda}{n_i})_+\ for\ all\ i=1,2,...,p$$

We want to minimize

$$L = \frac{1}{2}||\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda||\boldsymbol{\beta}_0|| = \frac{1}{2}(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda||\boldsymbol{\beta}||_0 = L_1 + L_2$$

where $L_1 = \frac{1}{2}(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$, $L_2 = \lambda||\boldsymbol{\beta}||_0$.

Case 1:

Here we view the optimization problem as a case in linear regression. The L_1 is exactly the $RSS/2$ in this case. So we compare the increment of L_1 when L_2 takes different values. We denote z as the number of non-zero elements in $\boldsymbol{\beta}$.
(1) Consider the case we have no constraint on z. Thus we only have to minimize L_1. By the knowledge of linear regression, we know the unique minimizer is $\hat{\boldsymbol{\beta}}_{\boldsymbol{ols}} = (\mathbf{X^TX})^{-1}\mathbf{XY}$. Assume there are m zero elements in $\hat{\boldsymbol{\beta}}_{\boldsymbol{ols}}$ where $0 \leq m \leq p$
(2) Consider the case we have constraint on z: $z = i$, where $i = 0, 1, 2, ..., m$. Obviously, among these cases the L can be minimized if and only if $i = m$. So, $z = m$ and $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}_{\boldsymbol{ols}}$ is the minimizer of L when $0 \leq z \leq m$. (3) Consider the case that we have constraint on x: $z = m+1$. Then we have to take one more non-zero element in $\boldsymbol{\beta}$ to be zero. Suppose we take $\hat{\beta}_l \neq 0$ to be 0. Then we obtain

$$2L_1 - SSE(\beta_1, ..., \beta_{l-1}, \beta_{l+1}, ..., \beta_p) = SSR(\beta_l)$$

by the columns in $\mathbf{X}$ are orthogonal to each other. Additionally,

$$SSR(\beta_l) = \mathbf{Y}^T(\mathbf{H} - \mathbf{H_l})\mathbf{Y}$$

where $\mathbf{H} = \mathbf{X}(\mathbf{X^TX})^{-1}\mathbf{X} = \sum_{i=1}^{p} \frac{1}{n_i}\mathbf{x_{(i)}}\mathbf{x_{(i)}^T}$, $\mathbf{H_l} = \sum_{i \neq j} \mathbf{x_{(i)}}\mathbf{x_{(i)}^T}$, $\hat{\beta}_l = \frac{1}{n_l}\mathbf{x_l}\mathbf{Y}$. Thus, we can simplify the second equation as:

$$SSR(\beta_l) = n_l\hat{\beta}_l^2$$

Thus, by taking $\hat{\beta}_l$ as 0, there is $\frac{n_l\hat{\beta}_l^2}{2}$ increment on L_1, λ decrement on L_2. Obviously, if the increment of L_1 is larger than the decrement L_2, we should not take $\hat{\beta}_l$ as 0; conversely, if the increment of L_1 is less than the decrement of L_2, taking $\hat{\beta}_l$ as 0 can lessen the L.
(4) As we discussed, if there is still at least one element in $\boldsymbol{\beta_k}$ that satisfies that $\frac{n_k\hat{\beta}_k^2}{2} \leq \lambda$, we can keep reducing L by taking $\boldsymbol{\beta_k}$ as 0 until all remain non-zero elements in $\hat{\beta}$ do not satisfy $\frac{n_k\hat{\beta}_k^2}{2} \leq \lambda$. Then we can minimize L.

Over all, the $\boldsymbol{\beta}$ that minimized L is:

$$\hat{\beta}_i = \hat{\beta}_{ols,i}\mathbb{I}_{|\hat{\beta}_{ols,i}| > \frac{\lambda'}{\sqrt{n_i}}} \; for \; all \; i = 1, ..., p$$

Case 2:

Here we use the properties of subderivative. Taking subderivative of L, we obtain

$$\frac{\partial L}{\partial \beta_j} = \begin{cases} \{n_j\beta_j - \mathbf{x_{(j)}^T}\mathbf{Y} + \lambda\} & \text{if } \beta_j > 0 \\ [n_j\beta_j - \mathbf{x_{(j)}^T}\mathbf{Y} - \lambda, n_j\beta_j - \mathbf{x_{(j)}^T}\mathbf{Y} + \lambda] & \text{if } \beta_j = 0 \\ \{n_j\beta_j - \mathbf{x_{(j)}^T}\mathbf{Y} - \lambda\} & \text{if } \beta_j < 0 \end{cases}$$

Because β_j minimize L if and only if $0 \in \frac{\partial L}{\partial \beta_j}$ and $\mathbf{X}$ is orthogonal, we get:

$$\hat{\beta}_j = \begin{cases} \frac{\mathbf{x_{(j)}^T}\mathbf{Y} + \lambda}{n_j} & \text{if } \hat{\beta}_j < 0 \\ 0 & \text{if } \hat{\beta}_j = 0 \\ \frac{\mathbf{x_{(j)}^T}\mathbf{Y} - \lambda}{n_j} & \text{if } \hat{\beta}_j > 0 \end{cases}$$

Here, $\hat{\boldsymbol{\beta}}_{ols} = (\mathbf{X^TX})^{-1}\mathbf{X^TY} = diag(1/n_1, ..., 1/n_p)X^TY$, so $\hat{\beta}_{ols,j} = \frac{\mathbf{x_{(j)}^T}\mathbf{Y}}{n_j}$. Then the solution of $\hat{\beta}_j$ can be simplified as:

$$\hat{\beta}_i = sign(\hat{\beta_{ols,i}})(|\hat{\beta_{ols,i}}| - \frac{\lambda}{n_i})_+ \; for \; all \; i = 1, 2, ..., p$$

n_1	n_2	n_3	d_1	d_2	d_3	noise	CER (mode 1)	CER (mode 2)	CER (mode 3)
40	40	40	3	5	4	4	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	40	40	3	5	4	8	$\mathbf{0}(\mathbf{0})$	0.0095(0.0247)	0.0021(0.0145)
40	40	40	3	5	4	12	0.0038(0.0138)	0.0331(0.0453)	0.0222(0.0520)
40	40	80	3	5	4	4	$\mathbf{0}(\mathbf{0})$	0.0017(0.0121)	$\mathbf{0}(\mathbf{0})$
40	40	80	3	5	4	8	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	40	80	3	5	4	12	$\mathbf{0}(\mathbf{0})$	$0.0257(0.0380)$	$0.0026(0.0064)$
40	40	40	4	4	4	4	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	40	40	4	4	4	8	0.0023(0.0165)	0.0034(0.0239)	$\mathbf{0}(\mathbf{0})$
40	40	40	4	4	4	12	0.0519(0.0744)	0.0414(0.0697)	0.0297(0.0644)
40	40	80	4	4	4	4	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	40	80	4	4	4	8	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	40	80	4	4	4	12	0.0132(0.0405)	0.0106(0.0366)	0.0043(0.0168)

Table 1: Given the true d_1, d_2, d_3, the simulation results is calculated across 50 tensors each time.

Dimensions (d_1, d_2, d_3)	True clustering sizes (R_1, R_2, R_3)	Noise (σ)	Estimated clustering sizes $(\hat{R}_1, \hat{R}_2, \hat{R}_3)$
$(40, 40, 40)$	$(4, 4, 4)$	4	$(\mathbf{4},\ \mathbf{4},\ \mathbf{4}) \pm (0,\ 0,\ 0)$
$(40, 40, 40)$	$(4, 4, 4)$	8	$(\mathbf{3.94},\ \mathbf{3.96},\ \mathbf{3.96}) \pm (0.03,\ 0.03,\ 0.03)$
$(40, 40, 40)$	$(4, 4, 4)$	12	$(3.08,\ 3.12,\ 3.12) \pm (0.10, 0.10, 0.10)$
$(40, 40, 80)$	$(4, 4, 4)$	4	$(\mathbf{4},\ \mathbf{4},\ \mathbf{4}) \pm (0,\ 0,\ 0)$
$(40, 40, 80)$	$(4, 4, 4)$	8	$(\mathbf{4},\ \mathbf{4},\ \mathbf{4}) \pm (0,\ 0,\ 0)$
$(40, 40, 80)$	$(4, 4, 4)$	12	$(\mathbf{3.96},\ \mathbf{3.96},\ 3.92) \pm (0.04, 0.04, 0.04)$
$(40, 40, 40)$	$(2, 3, 4)$	4	$(\mathbf{2},\ \mathbf{3},\ \mathbf{4}) \pm (0,\ 0,\ 0)$
$(40, 40, 40)$	$(2, 3, 4)$	8	$(\mathbf{2},\ \mathbf{3},\ \mathbf{3.96}) \pm (0,\ 0,\ 0.03)$
$(40, 40, 40)$	$(2, 3, 4)$	12	$(\mathbf{2},\ \mathbf{2.96},\ 3.60) \pm (0,\ 0.05,\ 0.09)$

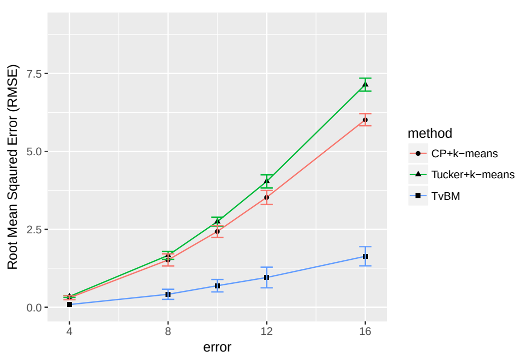
Table 2: The simulation results across 50 tensors each time from estimating the d_1, d_2, d_3. Highlight estimates that is no significant away from the truth based on a Z test.

n_1	n_2	n_3	d_1	d_2	d_3	noise	overall accuracy	estimated d_1	estimated d_2	estimated d_3
40	40	40	3	5	4	4	**1**	3(0)	5(0)	4(0)
40	40	40	3	5	4	8	0.74	3(0)	4.76(0.0610)	3.98(0.02)
40	40	40	3	5	4	12	0.02	2.8(0.0571)	3.58(0.1072)	3.3(0.0915)
40	40	40	4	4	4	4	**1**	4(0)	4(0)	4(0)
40	40	40	4	4	4	8	0.88	3.94(0.0339)	3.96(0.0280)	3.96(0.0280)
40	40	40	4	4	4	12	0.04	3.08(0.0983)	3.12(0.1016)	3.12(0.0975)
40	40	80	4	4	4	4	**1**	4(0)	4(0)	4(0)
40	40	80	4	4	4	8	1	4(0)	4(0)	4(0)
40	40	80	4	4	4	12	0.78	3.9(0.0429)	3.92(0.0388)	3.96(0.04)

Table 3: The simulation results across 50 tensors each time from estimating the d_1, d_2, d_3.

n_1	n_2	n_3	noise	CER(mode 1)	CER(mode 2)	CER(mode3)
40	40	40	4	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	40	40	8	$\mathbf{0}(\mathbf{0})$	0.0136(0.0226)	0.0005(0.0036)
40	40	40	12	0.0365(0.0789)	0.12(0.0878)	0.0802(0.1009)
40	45	50	4	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$	$\mathbf{0}(\mathbf{0})$
40	45	50	8	$\mathbf{0}(\mathbf{0})$	0.0027(0.0121)	$\mathbf{0}(\mathbf{0})$
40	45	50	12	0.0158(0.0489)	0.0641(0.0629)	0.0336(0.0647)

Table 4: The CERs over 50 simulated tensors ($d_1 = 3, d_2 = 5, d_3 = 4$) each time.


Root Mean Sqaured Error (RMSE)
0.0
2.5
5.0
7.5
4
8
12
16
error
method
CP+k−means
Tucker+k−means
TvBM