Supplements for "Exponential tensor regression with covariates on multiple modes"

1 Proofs

Proof of Theorem 4.1. Define $\ell(\mathcal{B}) = \mathbb{E}(\mathcal{L}_{\mathcal{Y}}(\mathcal{B}))$, where the expectation is taken with respect to $\mathcal{Y} \sim \mathcal{B}_{\text{true}}$ under the model with true parameter $\mathcal{B}_{\text{true}}$. We first prove the following two conclusions:

C1. There exists two positive constants C_1, $C_2 > 0$, such that, with probability at least $1 - \exp(-C_1 \log K \sum_k p_k)$, the stochastic deviation, $\mathcal{L}_{\mathcal{Y}}(\mathcal{B}) - \ell(\mathcal{B})$, satisfies

$$|\mathcal{L}_{\mathcal{Y}}(\mathcal{B}) - \ell(\mathcal{B})| = |\langle \mathcal{E}, \; \mathcal{B} \times_1 \boldsymbol{X}_1 \times_2 \cdots \times_K \boldsymbol{X}_K \rangle| \leq C_2 \|\mathcal{B}\|_F \log K \sqrt{\frac{\prod_k r_k}{\max_k r_k} \sum_k p_k}.$$

C2. The inequality $\ell(\hat{\mathcal{B}}) - \ell(\mathcal{B}_{\text{true}}) \leq -\frac{L}{2}\|\hat{\Theta} - \Theta^{\text{true}}\|_F^2$ holds, where $L > 0$ is the lower bound for $\min_{|\theta| \leq \alpha} |b''(\theta)|$.

To prove C1, we note that the stochastic deviation can be written as:

$$\begin{aligned}
\mathcal{L}_{\mathcal{Y}}(\mathcal{B}) - \ell(\mathcal{B}) &= \langle \mathcal{Y} - \mathbb{E}(\mathcal{Y}|\mathcal{X}), \; \Theta(\mathcal{B}) \rangle \\
&= \langle \mathcal{Y} - b'(\Theta^{\text{true}}), \; \Theta \rangle \\
&= \langle \mathcal{E} \times_1 \boldsymbol{X}_1^T \times_2 \cdots \times_K \boldsymbol{X}_K^T, \; \mathcal{B} \rangle,
\end{aligned} \tag{1}$$

where $\mathcal{E} = [\![\varepsilon_{i_1,\ldots,i_K}]\!] \overset{\text{def}}{=} \mathcal{Y} - b'(\Theta^{\text{true}})$. Based on Lemma 1, $\varepsilon_{i_1,\ldots,i_K}$ is sub-Gaussian-(ϕU). Let $\check{\mathcal{E}} \overset{\text{def}}{=} \mathcal{E} \times_1 \boldsymbol{X}_1^T \times_2 \cdots \times_K \boldsymbol{X}_K^T$. By the property of sub-Gaussian r.v's, $\check{\mathcal{E}}$ is a $(p_1, \ldots, p_K)$-dimensional sub-Gaussian tensor with parameter bounded by $C_2 = \phi U c_2^K$. Here $c_2 > 0$ is the upper bound of $\sigma_{\max}(\boldsymbol{X}_k)$. Applying Cauchy-Schwarz inequality to (1) yields

$$|\mathcal{L}_{\mathcal{Y}}(\mathcal{B}) - \ell(\mathcal{B})| \leq \|\check{\mathcal{E}}\|_2 \|\mathcal{B}\|_*, \tag{2}$$

where $\|\cdot\|_2$ denotes the tensor spectral norm and $\|\cdot\|_*$ denotes the tensor nuclear norm. The nuclear norm $\|\mathcal{B}\|_*$ is bounded by $\|\mathcal{B}\|_* \leq \sqrt{\frac{\prod_k r_k}{\max_k r_k}} \|\mathcal{B}\|_F$ (c.f. [1, 2]). The spectral norm $\|\check{\mathcal{E}}\|_2$ is bounded by $\|\check{\mathcal{E}}\|_2 \leq C_1 U c^K \log K \sqrt{\sum_k p_k}$ with probability at least $1 - \exp(-C_2 \log K \sum_k p_k)$ (c.f. [1, 3]). Combining these two bounds with (2), we have, with probability at least $1 - \exp(-C_2 \log K \sum_k p_k)$,

$$|\mathcal{L}_{\mathcal{Y}}(\mathcal{B}) - \ell(\mathcal{B})| \leq C_1 U c_2^K \|\mathcal{B}\|_F \log K \sqrt{\frac{\prod_k r_k}{\max_k r_k} \sum_k p_k}.$$

Next we prove C2. Applying Taylor expansion to $\ell(\mathcal{B})$ around $\mathcal{B}_{\text{true}}$,

$$\ell(\mathcal{B}) = \ell(\mathcal{B}_{\text{true}}) - \frac{1}{2}\text{vec}(\mathcal{B} - \mathcal{B}_{\text{true}})^T \mathcal{H}_{\mathcal{Y}}(\check{\mathcal{B}})\text{vec}(\mathcal{B} - \mathcal{B}_{\text{true}}), \tag{3}$$

where $\mathcal{H}_{\mathcal{Y}}(\check{\mathcal{B}})$ is the (non-random) Hession of $\frac{\partial \ell^2(\mathcal{B})}{\partial^2 \mathcal{B}}$ evaluated at $\check{\mathcal{B}} = \alpha\text{vec}(\alpha \mathcal{B} + (1 - \alpha)\mathcal{B}_{\text{true}})$ for some $\alpha \in [0, 1]$. Recall that $b''(\theta) = \text{Var}(y|\theta)$, because $y \in \mathbb{R}$ follows the exponential family

distribution with function $b(\cdot)$. By chain rule and the fact that $\Theta = \Theta(\mathcal{B}) = \mathcal{B} \times_1 \boldsymbol{X}_1 \cdots \times_K \boldsymbol{X}_K$, the equation (3) implies that

$$\ell(\mathcal{B}) - \ell(\mathcal{B}_{\text{true}}) = -\frac{1}{2} \sum_{i_1,\dots,i_K} b''(\breve{\theta}_{i_1,\dots,i_K})(\theta_{i_1,\dots,i_K} - \theta_{\text{true},i_1,\dots,i_K})^2 \leq -\frac{L}{2} \|\Theta - \Theta^{\text{true}}\|_F^2, \qquad (4)$$

holds for all $\mathcal{B} \in \mathcal{P}$, provided that $\min_{|\theta| \leq \alpha} |b''(\theta)| \geq L > 0$. In particular, the inequality (4) also applies to the constrained MLE $\hat{\mathcal{B}}$. So we have

$$\ell(\hat{\mathcal{B}}) - \ell(\mathcal{B}_{\text{true}}) \leq -\frac{L}{2} \|\hat{\Theta} - \Theta^{\text{true}}\|_F^2. \qquad (5)$$

Now we have proved both C1 and C2. Note that $\mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{B}}) - \mathcal{L}_{\mathcal{Y}}(\mathcal{B}_{\text{true}}) \geq 0$ by the definition of $\hat{\mathcal{B}}$, This implies that

$$\begin{aligned}
0 &\leq \mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{B}}) - \mathcal{L}_{\mathcal{Y}}(\mathcal{B}_{\text{true}}) \\
&\leq \left(\mathcal{L}_{\mathcal{Y}}(\hat{\mathcal{B}}) - \ell(\hat{\mathcal{B}}) \right) - (\mathcal{L}_{\mathcal{Y}}(\mathcal{B}_{\text{true}}) - \ell(\mathcal{B}_{\text{true}})) + \left(\ell(\hat{\mathcal{B}}) - \ell(\mathcal{B}_{\text{true}}) \right) \\
&\leq \langle \mathcal{E},\ \Theta - \Theta^{\text{true}} \rangle - \frac{L}{2} \|\hat{\Theta} - \Theta^{\text{true}}\|_F^2,
\end{aligned}$$

where the second line follows from (5). Therefore,

$$\begin{aligned}
\|\hat{\Theta} - \Theta^{\text{true}}\|_F &\leq \frac{2}{L} \langle \mathcal{E},\ \frac{\hat{\Theta} - \Theta^{\text{true}}}{\|\hat{\Theta} - \Theta^{\text{true}}\|_F} \rangle \\
&\leq \frac{2}{L} \sup_{\Theta: \|\Theta\|_F = 1, \Theta = \mathcal{B} \times_1 \boldsymbol{X}_1 \times_2 \cdots \times_K \boldsymbol{X}_K} \langle \mathcal{E},\ \Theta \rangle \\
&\leq \frac{2}{L} \sup_{\mathcal{B} \in \mathcal{P}: \|\mathcal{B}\|_F \leq \prod_k \sigma_{\min}^{-1}(\boldsymbol{X}_k)} \langle \mathcal{E},\ \mathcal{B} \times_1 \boldsymbol{X}_1 \times_2 \cdots \times_K \boldsymbol{X}_K \rangle. \qquad (6)
\end{aligned}$$

Combining (6) with C1 yields the desired conclusion.

$\square$

Lemma 1 (sub-Gaussian residual). *Define the residual tensor* $\mathcal{E} = [\![\varepsilon_{i_1,\dots,i_K}]\!] = \mathcal{Y} - b'(\Theta) \in \mathbb{R}^{d_1 \times \cdots \times d_K}$. *Under the Assumption A2,* $\varepsilon_{i_1,\dots,i_K}$ *is a sub-Gaussian random variable with sub-Gaussian parameter bounded by* ϕU, *for all* $(i_1, \dots, i_K) \in [d_1] \times \cdots \times [d_K]$.

Proof. The proof is similar to Lemma 3 in [4]. For ease of presentation, we drop the subscript $(i_1, \dots, i_K)$ and simply write ε $(= y - b'(\theta))$. For any given $t \in \mathbb{R}$, we have

$$\begin{aligned}
\mathbb{E}(\exp(t\varepsilon|\theta) &= \int c(x) \exp\left(\frac{\theta x - b(\theta)}{\phi} \right) \exp\left(t(x - b'(\theta)) \right) dx \\
&= \int c(x) \exp\left(\frac{(\theta + \phi t)x - b(\theta + \phi t) + b(\theta + \phi t) - b(\theta) - \phi t b'(\theta)}{\phi} \right) dx \\
&= \exp\left(\frac{b(\theta + \phi t) - b(\theta) - \phi t b'(\theta)}{\phi} \right) \\
&\leq \exp\left(\frac{\phi U t^2}{2} \right),
\end{aligned}$$

where $c(\cdot)$ and $b(\cdot)$ are known functions in the exponential family corresponding to y. Therefore, ε is sub-Gaussian-(ϕU).

$\square$

Proof of Theorem 4.2. The proof is similar to [5]. We sketch the main steps here for completeness. Recall that $\ell(\mathcal{B}) = \mathbb{E}(\mathcal{L}_{\mathcal{Y}}(\mathcal{B}))$. By the definition of KL divergence, we have that,

$$\ell(\hat{\mathcal{B}}) = \ell(\mathcal{B}_{\text{true}}) - \sum_{(i_1,\ldots,i_K)} KL(\theta_{\text{true},i_1,\ldots,i_K}, \hat{\theta}_{i_1,\ldots,i_K})$$
$$= \ell(\mathcal{B}_{\text{true}}) - \text{KL}(\mathbb{P}_{\mathcal{Y}_{\text{true}}}, \mathbb{P}_{\hat{y}}),$$

where $\mathbb{P}_{\mathcal{Y}_{\text{true}}}$ denotes the distribution of $\mathcal{Y}|\mathcal{X}$ with true parameter $\mathcal{B}_{\text{true}}$, and $\mathbb{P}_{\hat{y}}$ denotes the distribution with estimated parameter $\hat{\mathcal{B}}$. Therefore

$$\text{KL}(\mathbb{P}_{\mathcal{Y}_{\text{true}}}, \mathbb{P}_{\hat{y}}) = \ell(\mathcal{B}_{\text{true}}) - \ell(\hat{\mathcal{B}})$$
$$= \frac{1}{2} \sum_{i_1\ldots,i_K} b''(\check{\theta}_{i_1,\ldots,i_K})(\theta_{i_1,\ldots,i_K} - \theta_{\text{true},i_1,\ldots,i_K})^2$$
$$\leq \frac{U}{2} \|\Theta - \Theta^{\text{true}}\|_F^2$$
$$\leq \frac{U}{2} c_2^{2K} \|\mathcal{B} - \mathcal{B}_{\text{true}}\|_F^2,$$

where the second line comes from (3), and $c_2 > 0$ is the upper bound for the $\sigma_{\max}(\boldsymbol{X}_k)$. The result then follows from Theorem 4.1. $\qquad\square$

Proof of Proposition 1. Waiting for the proof. $\qquad\square$

2 Numerical implementation

2.1 Alternating Algorithm

The detailed alternating algorithm is organized in Algorithm 1.

Algorithm 1 Generalized tensor response regression with covariates on multiple modes

---
Input: Response tensor $\mathcal{Y} \in \mathbb{R}^{d_1 \times \cdots \times d_K}$, covariate matrices $\boldsymbol{X}_k \in \mathbb{R}^{d_k \times p_k}$ for $k = 1,\ldots,K$, target Tucker rank $\boldsymbol{r} = (r_1,\ldots,r_K)$, link function f, infinity norm bound α
Output: Low-rank estimation for the coefficient tensor $\mathcal{B} \in \mathbb{R}^{p_1 \times \cdots \times p_K}$.
 1: Calculate $\check{\mathcal{B}} = \mathcal{Y} \times_1 \left[(\boldsymbol{X}_1^T \boldsymbol{X}_1)^{-1} \boldsymbol{X}_1^T\right] \times_2 \cdots \times_K \left[(\boldsymbol{X}_K^T \boldsymbol{X}_K)^{-1} \boldsymbol{X}_K^T\right]$.
 2: Initialize the iteration index $t = 0$. Initialize the core tensor $\mathcal{C}^{(0)}$ and factor matrices $\boldsymbol{M}_k^{(0)} \in \mathbb{R}^{p_k \times r_k}$ via rank-$\boldsymbol{r}$ Tucker approximation of $\check{\mathcal{B}}$, in the least-square sense.
 3: **while** the relative increase in objective function $\mathcal{L}_{\mathcal{Y}}(\mathcal{B})$ is less than the tolerance **do**
 4:     Update iteration index $t \leftarrow t + 1$.
 5:     **for** $k = 1$ to K **do**
 6:         Obtain the factor matrix $\boldsymbol{M}_k^{(t+1)} \in \mathbb{R}^{p_k \times r_k}$ by solving p_k separate GLMs with link function f.
 7:         Update the columns of $\boldsymbol{M}_k^{(t+1)}$ by Gram-Schmidt orthogonalization.
 8:     **end for**
 9:     Obtain the core tensor $\mathcal{C}^{(t+1)} \in \mathbb{R}^{r_1 \times \cdots \times r_K}$ by solving a GLM with $\text{vec}(\mathcal{Y})$ as response, $\odot_{k=1}^K [\boldsymbol{X}_k \boldsymbol{M}_k^{(t)}]$ as covariates, and f as link function. Here $\odot$ denotes the Khatri-Rao product of matrices.
10:     Rescale the core tensor subject to the infinity norm constraint.
11:     Update $\mathcal{B}^{(t+1)} \leftarrow \mathcal{C}^{(t+1)} \times_1 \boldsymbol{M}_1^{(t+1)} \times_2 \cdots \times_K \boldsymbol{M}_K^{(t+1)}$.
12: **end while**

2.2 Time complexity

The computational complexity of our tensor regression model is $O(d^3 + d)$ for each loop of iterations, where $d = \prod_k d_k$ is the total size of the response tensor. More precisely, the update of core tensor costs $O(r^3 d^3)$, where $r = \sum_k r_k$ is the total size of the core tensor. The update of factor matrix $\boldsymbol{M}_k$ involves solving p_k separate GLMs. Solving those GLMs requires $O(r_k^3 p_k + p_k r_k^3 d d_k^{-1})$, and therefore the cost for updating K factors in total is $O(\sum_k r_k^3 p_k d_k + d \sum_k r_k^3 p_k d_k^{-1}) \approx O(\sum p_k d_k + d) \approx O(d)$.

3 Simulation

3.1 Detailed simulation setting

In simulations, we used linear predictor simulated from $\mathcal{U} = [\![u_{ijk}]\!] = \mathcal{B} \times \{\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{X}_3\}$. Here, we introduce the detailed setting to generate $\mathcal{U}$. The coefficient tensor $\mathcal{B}$ was generated using the Tucker factor representation $\mathcal{B} = \mathcal{C} \times \{\boldsymbol{M}_1, \boldsymbol{M}_2, \boldsymbol{M}_3\}$, where both the core tensor $\mathcal{C}$ and factor matrices $\{\boldsymbol{M}_k\}$ were drawn i.i.d. from Uniform[-1,1]. The covariate matrix $\boldsymbol{X}_k$ was either an identity matrix(i.e. no covariate available) or Gaussian random matrix with i.i.d. entries from $N(0, \sigma_k)$. We set $\sigma_k = d_k^{1/2}$ to ensure the singular values of $\boldsymbol{X}_k$ are bounded as d_k increases. The linear predictor $\mathcal{U}$ was also scaled such that $\mathcal{U}\| = \mathcal{U}\|_{\max} 1$.

3.2 Simulation for rank selection

We provide the experiment results for assessing our BIC criterion (9). We consider the balanced situation where $d_k = d$, $p_k = 0.4 d_k$ for $k = 1, 2, 3$. We set $\alpha = 10$ and consider various combinations of dimension d and rank $\boldsymbol{r} = (r_1, r_2, r_3)$. For each combination, we simulate tensor data following Gaussian, Bernoulli, and Poisson models. We then minimize BIC using a grid search over three dimensions. The hyper-parameter α is set to infinity in the fitting, which essentially imposes no prior on the coefficient magnitude. Table S1 reports the selected rank averaged over $n_{\mathrm{sim}} = 30$ replicates for Gaussian and Poisson models. We found that when $d = 20$, the selected rank is slightly smaller than the true rank, and the accuracy improves immediately when the dimension increases to $d = 40$. This agrees with our expectation, as in tensor regression, the sample size is related to the number of entries. A larger d implies a larger sample size, so the BIC selection becomes more accurate.

True Rank	Dimension (Gaussian tensors)		Dimension (Poisson tensors)	
$\boldsymbol{r}$	$d = 20$	$d = 40$	$d = 20$	$d = 40$
(3, 3, 3)	(2.1, 2.0, 2.0)	(**3**, **3**, **3**)	(2.0, 2.2, 2.1)	(**3**, **3**, **3**)
(4, 4, 6)	(3.2, 3.1, 5.0)	(**4**, **4**, **6**)	(**4.0**, **4.0**, 5.2)	(**4**, **4**, **6**)
(6, 8, 8)	(5.1, 7.0, 6.9)	(**6**, **8**, **8**)	(5.0, 6.1, 7.1)	(**6**, **8**, **8**)

Supplementary Table S1: Rank selection via BIC. Bold number indicates no significant difference between the estimate and the ground truth, based on a z-test with a level 0.05.

# 4 Additional results for real data analysis

4.1 HCP data analysis

Supplement Figure S1 compares the estimated coefficients from our method (tensor regression) with those from classical GLM approach. A classical GLM is to regress the brain edges, one at a

time, on the individual-level covariates, and this logistic model is repeatedly fitted for every edge $\in [68] \times [68]$. As we can see in the figure, our tensor regression shrinkages the coefficients towards center, thereby enforcing the sharing between coefficient entries.

4.2 Nations data analysis

We apply our tensor regression model to the *Nations* data. The multi-relationship networks are organized into a $14 \times 14 \times 56$ binary tensor, with each entry indicating the presence or absence of a connection, such as "sending tourist to", "export", "import", between countries. The 56 relations span the fields of politics, economics, military, religion, etc. The BIC criterion suggests a rank $\boldsymbol{r} = (4, 4, 4)$ for the coefficient tensor $\mathcal{B} \in \mathbb{R}^{6 \times 6 \times 56}$.

To investigate the effects of dyadic attributes towards connections, we depicted the estimated coefficients $\hat{\mathcal{B}} = [\![\hat{b}_{ijk}]\!]$ for several relation types (Supplement Figure S2). Note that entries $\hat{b}_{ijk}$ can be interpreted as the contribution, at the logit scale, of covariate pair (i, j) (ith covariate for the "sender" country and jth covariate for the "receiver" country) towards the connection of relation k. Several interesting findings emerge from the observation. We found that relations belonging to a same cluster tend to have similar covariate effects. For example, the relations *warnings* and *ecnomicaid* are classified into Cluster II, and both exhibit similar covariate pattern (Supplement Figure S2a-b). Moreover, the majority of the diagonal entries $\hat{\mathcal{B}}(i, i, k)$ positively contribute to the connection. This suggests that countries with coherent attributes tend to interact more often than others. We also found that the *constitutional* attribute is an important predictor for the *commonbloc* relation, whereas the effect is weaker for other relations (Supplement Figure S2d). This is not surprising, as the block partition during Cold War is associated with the *constitutional* attribute.
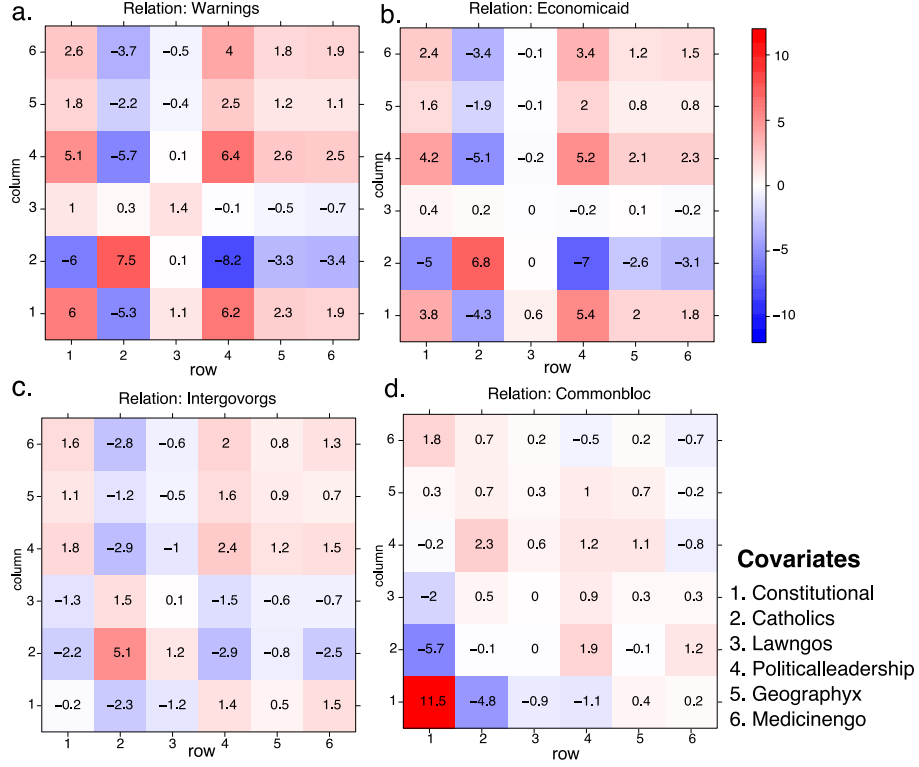
Supplementary Figure S2: Effect estimation in the *Nations* data. Panels (a)-(d) represent the estimated effects of country-level attributes towards the connection probability, for relations *warnning*, *economicaid*,*intergovorg*, and *commonblock*, respectively.

Supplement table S2 summarizes the K-means clustering of the 56 relations based on the 3$^{\mathrm{rd}}$ mode factor $\boldsymbol{M}_3 \in \mathbb{R}^{56 \times 4}$ in the tensor regression model.

Cluster I	officialvisits, intergovorgs, militaryactions, violentactions, duration, negativebehavior, boycottembargo, aidenemy, negativecomm, accusation, protestsunoffialacts, nonviolentbehavior, emigrants, relexports, timesincewar, commonbloc2, rintergovorgs3, relintergovorgs
Cluster II	economicaid, booktranslations, tourism, relbooktranslations, releconomicaid, conferences, severdiplomatic, expeldiplomats, attackembassy, unweightedunvote, reltourism, tourism3, relemigrants, emigrants3, students, relstudents, exports, exports3, lostterritory, dependent, militaryalliance, warning
Cluster III	treaties, reltreaties, exportbooks, relexportbooks, weightedunvote, ngo, relngo, ngoorgs3, embassy, reldiplomacy, timesinceally, independence, commonbloc1
Cluster IV	commonbloc0, blockpositionindex

Supplementary Table S2: K-means clustering of relations based on factor matrix in the coefficient tensor.

6

Supplementary Figure S1: Comparison of coefficient estimation in the HCP data.
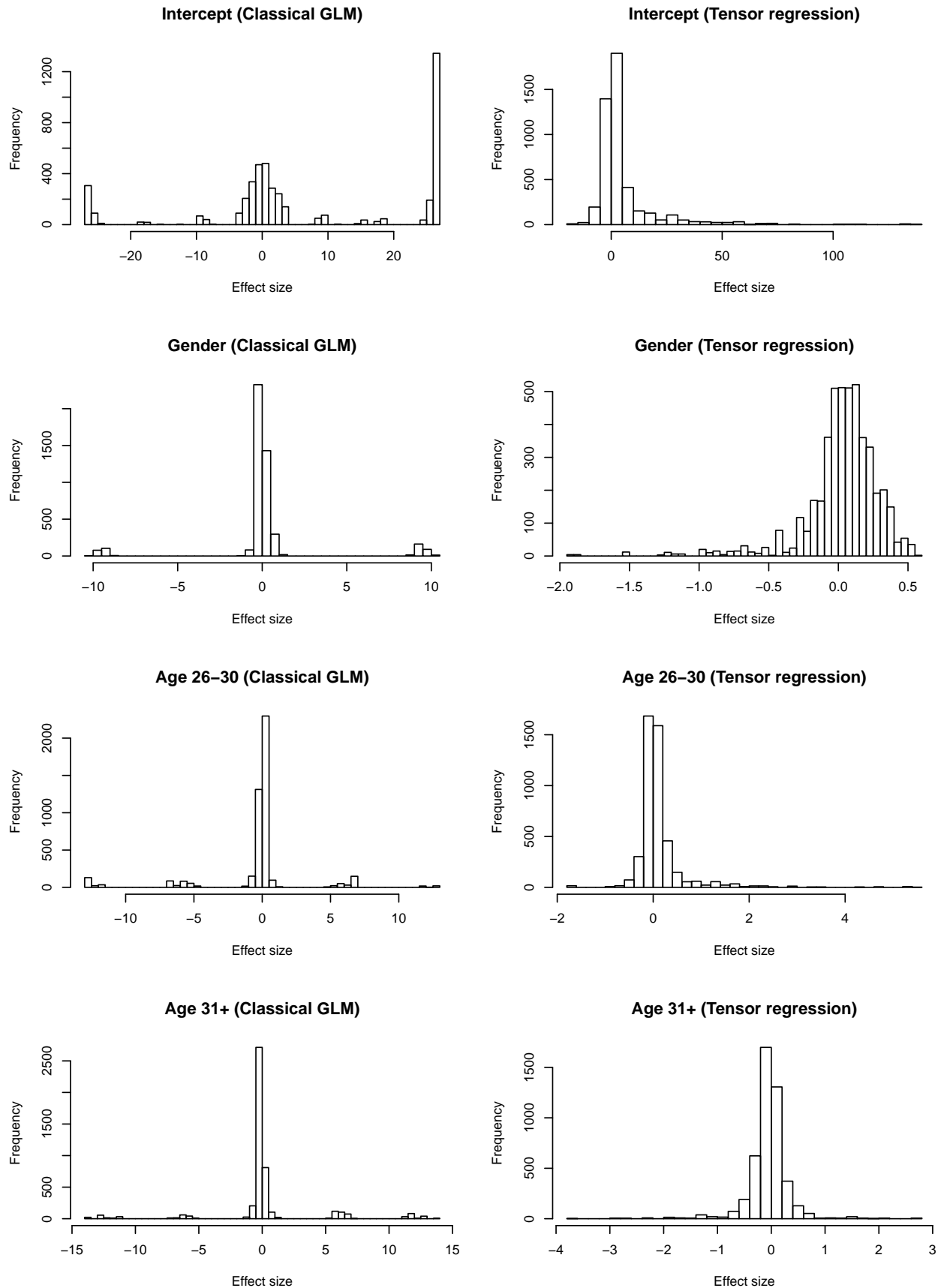
References

[1] Miaoyan Wang and Lexin Li. Learning from binary multiway data: Probabilistic tensor decomposition and its statistical optimality. *arXiv preprint arXiv:1811.05076*, 2018.

[2] Miaoyan Wang, Khanh Dao Duc, Jonathan Fischer, and Yun S Song. Operator norm inequalities between tensor unfoldings on the partition lattice. *Linear Algebra and Its Applications*, 520:44–66, 2017.

[3] Ryota Tomioka and Taiji Suzuki. Spectral norm of random tensors. *arXiv preprint arXiv:1407.1870*, 2014.

[4] Jianqing Fan, Wenyan Gong, and Ziwei Zhu. Generalized high-dimensional trace regression via nuclear norm regularization. *Journal of Econometrics*, 2019.

[5] Nicolai Baldin and Quentin Berthet. Optimal link prediction with matrix logistic regression. *arXiv preprint arXiv:1803.07054*, 2018.