Bayesian Tensor Regression: A Scalable Bayesian Framework in Neuroscience Applications

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Bayesian Tensor Regression

High Dimensional Regression

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Object Oriented Regression

• Answering complex inferential questions can lead to massive dimensional regression.

Detecting Voxels in Diseased Brain



Tensor predictor: Resting state fMRI for 550 people (some patients, some normal).

scalar predictors: volume of the brain, sex, smoking during pregnancy.

Response: Binary indicator whether diseased or not.











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- Efficient convex optimization algorithms (Hastie, 2003; Friedman, 2010) to produce point prediction for high dimensional regression.
- Unsatisfactory predictive uncertainty.

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Spike & Slab Prior (Computationally Inefficient)

 $\gamma_j \sim \pi \delta_0 + (1 - \pi)g$, g is a cont. density.



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Serious Drawbacks of Penalization and Shrinkage

- *p* = *p*₁ × *p*₂ × · · · *p*_D, each *p_i* = 64 typically, implies massive dimensional regression with close to half a million predictors ⇒ Infeasibility
- Misses out on wealth of information that the tensor valued brain images carry.
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Tensor Regression Model with PARAFAC Decomposition

Data Model

$$y = \langle \boldsymbol{X}, \boldsymbol{B} \rangle + \boldsymbol{z}' \boldsymbol{\gamma} + \epsilon, \epsilon \sim \mathrm{N}(0, \sigma^2)$$

rank-R PARAFAC decomposition of B for dimension reduction



For D > 3, need a better notation $\Rightarrow \boldsymbol{B} = \sum_{r=1}^{R} \beta_1^{(r)} \circ \cdots \circ \beta_D^{(r)}$ $\beta_j^{(r)} \in \mathscr{R}^{p_j}$, \circ denotes *outer product* between vectors.

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rank-R PARAFAC decomposition of *B* for dimension reduction Advantages

- ▶ Number of parameters needed to model is $R \sum_{j=1}^{D} p_j$ as opposed to $\prod_{j=1}^{D} p_j \Rightarrow$ Dimension Reduction.
- ► Keeps spatial structure of X intact ⇒ potentially better inference.

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$\psi(\cdot) = \text{convex penalty function}, \zeta = \text{tuning parameter}$

$$\arg\min_{\boldsymbol{\gamma},\boldsymbol{\beta}_{j}^{(r)}}\sum_{i=1}^{n}\left(y_{i}-\langle\boldsymbol{X}_{i},\boldsymbol{B}\rangle-\boldsymbol{z}_{i}^{\prime}\boldsymbol{\gamma}\right)^{2}+\zeta\left[\psi\left(\boldsymbol{\gamma}\right)+\sum_{r=1}^{R}\sum_{j=1}^{D}\psi\left(\boldsymbol{\beta}_{j}^{(r)}\right)\right]$$

Issues with Frequentist Tensor Regression (FTR)

- 1 Choice of *R* is adhoc.
- **2** Result depends heavily on the tuning parameter ζ . Choice of the tuning parameter is also uncertain.
- **3** Prediction and inference can be improved.

Multiway Shrinkage Prior for B (Guhaniyogi et al. 2015)



 $\beta_j^{(r)} \sim N(\mathbf{0}, \boldsymbol{W}_{jr} \tau \phi_r), \phi_r$'s rank specific parameters. Shrinkage across ranks: $(\phi_1, ..., \phi_R) \sim Dirichlet(\alpha_1, ..., \alpha_R).$



Multiway Dirichlet Generalized Double Pareto Prior (M-DGDP)



Shrinkage within every rank

 $w_{jr,k} \sim \operatorname{Exp}(\lambda_{jr}^2/2), \quad \lambda_{jr} \sim \operatorname{Ga}(a_{\lambda}, b_{\lambda}), \tau \sim IG(a_{\tau}, b_{\tau})$ Integrating out W_{jr}

$$\beta_{j,k}^{(r)}|\lambda_{jr},\phi_r,\tau \stackrel{i.i.d}{\sim} \mathrm{DE}(\lambda_{jr}/\sqrt{\phi_r\tau}), \ 1 \leq k \leq p_j,$$

i.e. $\beta_{i,k}^{(r)} | \phi_r, \tau$ marginally follows GDP shrinkage prior.

Bayesian Tensor Regression

General Theoretical Setup: Guhaniyogi et al., 2015



True Model
$$(f(y|\boldsymbol{B}_n^0) = N(\langle \boldsymbol{X}, \boldsymbol{B}_n^0 \rangle, \sigma^2))$$

Class of tensor reg. models fitted to the data

KL metric ball of radius ϵ around the truth

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KL metric ball of radius ϵ around the truth

$$\mathscr{B}_n = \left\{ \boldsymbol{B}_n : \frac{1}{n} \sum_{i=1}^n \mathsf{KL}(f(y_i | \boldsymbol{B}_n^0), f(y_i | \boldsymbol{B}_n)) < \epsilon \right\} \Rightarrow Neighborhood$$

Posterior Consistency

$$\Pi_n\left({\mathscr B}^{\mathsf{c}}_n
ight) o 0$$
 under ${oldsymbol B}^0_n$ a.s. as $n o\infty.$ (1)

 Π_n posterior distribution given y_1, \ldots, y_n .

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Posterior Consistency Results, Guhaniyogi et al. 2015

Theorem

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1 $\boldsymbol{B}_{n}^{0} = \sum_{r=1}^{R^{0}} \beta_{1,n}^{0(r)} \circ \cdots \circ \beta_{D,n}^{0(r)}$ follows rank- R^{0} decomposition. (Structure on the true coefficients)

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2 sup<sub>*l*=1,...,*p*_{*j*,*n*}
$$|\beta_{j,n,l}^{0(r)}| < \infty$$
, for all $j = 1, ..., D$; $r = 1, ..., R$.
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2 sup_{*l*=1,...,*p*_{*j*,*n*} $|\beta_{j,n,l}^{0(r)}| < \infty$, for all j = 1, ..., D; r = 1, ..., R. (Structure on the true coefficients)}

$$\boxed{I} \sum_{j=1}^{D} p_{j,n} \log(p_{j,n}) = o(n).$$
(Dimension of margins)

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Simulation Setup

Data Generation

$$y_i = \langle \boldsymbol{X}_i, \boldsymbol{B}^0 \rangle + \epsilon_i, \epsilon_i \sim N(0, \sigma_0^2), \ i = 1, ..., n$$

(i)
$$n = 1000$$

(ii) $\sigma_0^2 = 1$
(iii) B^0 is 64×64
(iv) $x_{i_1,i_2} \sim N(0,1) \forall i_1 = 1: 64, i_2 = 1: 64.$

Competitors

Frequentist Tensor Regression (FTR)

Vectorized Lasso (Lasso)

Results: True Tensor Coefficient are "Generated Shapes"



Bayesian Tensor Regression

Results: True Coefficients "Ready-made" Images









Bayesian Tensor Regression

Comparison with Competitors: Lower Mean Squared Error (MSE) with Excellent Coverage

Case	BTR	FTR	Lasso	VOX
Eagle	0.226 _{0.02}	0.354 _{0.03}	0.665 _{0.03}	> 0
Horse	0.278 _{0.01}	0.391 _{0.03}	0.888 _{0.01}	> 0
Eagle	0.085 _{0.00}	0.163 _{0.03}	0.097 _{0.00}	= 0
Horse	0.137 _{0.00}	0.2150.02	0.155 _{0.02}	= 0

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Coverage for M-DGDP is 0.94 and 0.92 respectively.

Simulated Response with Real Vector and Tensor Covariates

- $30 \times 30 \times 30$ MRI images (predictor tensor) for 550 individuals.
- Response is simulated as $y \sim N(\langle X, B^0 \rangle + z'\gamma, 1)$ for every individual.
- Three different rank-2 tensor coefficients are simulated with varying sparsity.

Case	BTR	FTR	Lasso
Cuse	DIR		Lusso
Case 1	0.13 _{0.01}	0.15 _{0.01}	0.15 _{0.01}
Case 2	0.20 _{0.01}	0.23 _{0.01}	0.24 _{0.01}
Case 3	0.17 _{0.01}	0.19 _{0.01}	0.19 _{0.01}

Brain Connectome Data Application

• Data are extracted from diffusion tensor imaging (DTI) for 109 individuals.

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- For each individual, brain connections are encoded by a 70×70 weighted adjacency matrix.
- The (*i*, *j*)-th entry of the matrix is the estimated number of fiber tracts connecting the *i*-th and *j*-th brain region.



Goal

Developing a predictive model of composite creativity index (CCI) based on neuronal connectivity.

Predictive Inference: Brain Connectome Data

• Response: Composite Creativity Index (CCI).

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Predictive Inference: Brain Connectome Data

- **Response:** Composite Creativity Index (CCI).
- Vector Predictor: 10 clinical covariates e.g. openness, agreeableness, conscientiousness.
- Tensor Predictor: 70 × 70 weighted adjacency matrix.
- Predictive inference of lasso and BTR with 10 folds of the data.

Method	avg(RMSE)	sd(RMSE)	avg(cov.)	sd(cov.)	avg(cor.)	sd(cor.)
Lasso	9.18	1.64	0.63	0.20	0.31	0.11
BTR	9.03	2.18	0.91	0.10	0.32	0.13

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Tensor Regression with M-DGDP prior

- A novel multiway shrinkage prior- R selection is automated,
- significantly better performance, excellent parametric and predictive coverage.

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- Supported by theoretical convergence results.

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Useful in Other Tensor Regression Framework? Nontrivial extension of BTR useful in providing a scalable framework for the brain activation study. Stay tuned....

• Supported by theoretical convergence results.

- Armagan, A., Dunson, D.B., and Lee, J. (2013), "Generalized Double Pareto Shrinkage," *Statistica Sinica*, 23, 119-143.
- Guhaniyogi, R., Qamar, S., and Dunson, D. B. (2015), "Bayesian Tensor Regression," *arXiv:1509.06490*.
- Zhou, H. (2013), "Tensor Regression with Applications in Neuroimaging Data Analysis," *Journal of the American Statistical Association*, **108**, 540-552.
- Zhou, H. and Li, Lexin (2014), "Regularized Matrix Regression," *Journal of the Royal Statistical Society, Series B*, **76**, 463-483.
- Carvalho, C.M., Polson, N.G., and Scott, J.G. (2009), "Handling Sparsity via The Horseshoe," *JMLR: W & CP*, 5, 73-80.

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