

Generalized Linear Model for a Spherical Response with Projection-based Inference

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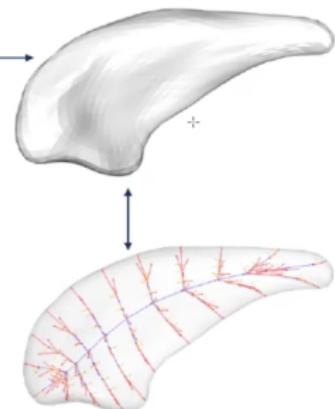
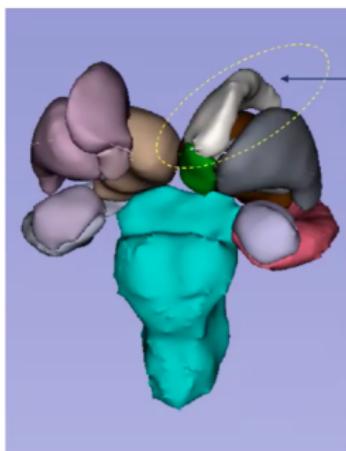
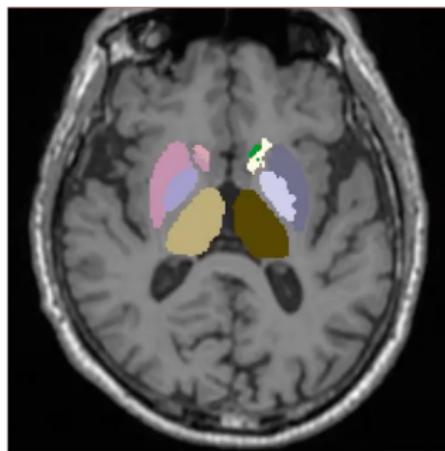
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Motivating data

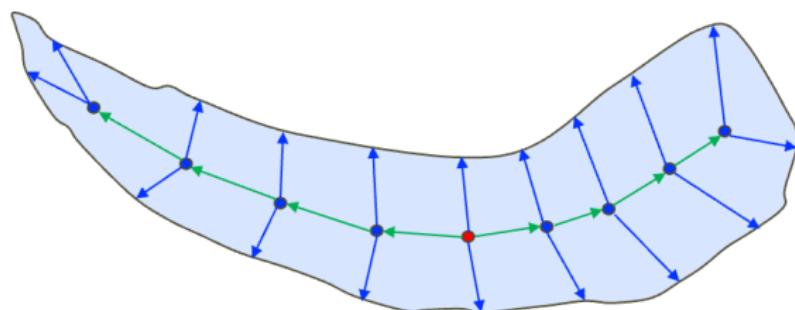
Shape data from a brain MRI

- From Brain MRI, we can obtain the shape of specific regions as 3D point cloud data in (x,y,z) coordinates. In our case, the shapes of hippocampus were collected.
- In this study, we aim test for shape differences in the **hippocampus**, derived from a brain MRI, between a **Parkinson's disease (PD)** group and a normal control group.



Data Representation

- However, 3d point cloud data originally poses significant analytical challenges, as the large number of points effectively creates a high-dimensional feature space.
- To address this, we transform the shape into a compressed representation using the locally parametrized discrete-skeletal representation (LP-ds-rep) method (Taheri and Schulz, 2021).
- Simply speaking, this transformation gives us key features that effectively capture the shape: the **centroid**, **connection vectors** forming the spine, and **spoke vectors** extending toward the shape's boundary.



Mathematical Formulation

- Connection and spoke vectors can be thought of as a direction times its length.
- Each data point can be considered an element of the following space:

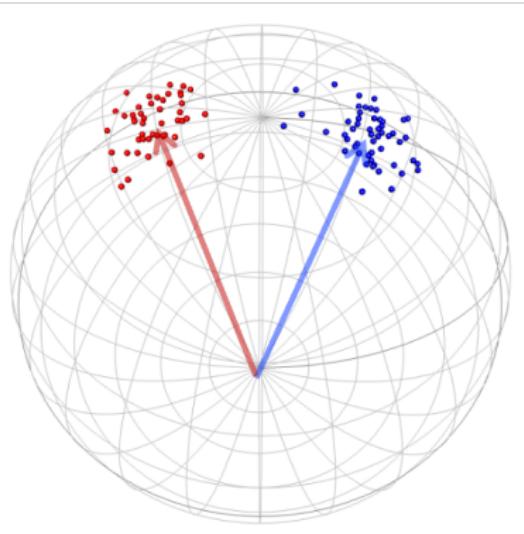
$$\underbrace{\mathbb{R}^3}_{\text{centroid}} \times \underbrace{(\mathbb{S}^2)^{n_c} \times (\mathbb{R}_+)^{n_c}}_{\text{connections}} \times \underbrace{(\mathbb{S}^2)^{n_s} \times (\mathbb{R}_+)^{n_s}}_{\text{spokes}}, \quad (1)$$

where $\mathbb{S}^{q-1} = \left\{ \mathbf{y} \in \mathbb{R}^q : \mathbf{y}^T \mathbf{y} = 1 \right\}$.

- In this work, we focus specifically on the spoke vectors. We propose a method to test for differences in a single spoke direction between the case and control groups.

The Two-Sample Problem on a Sphere

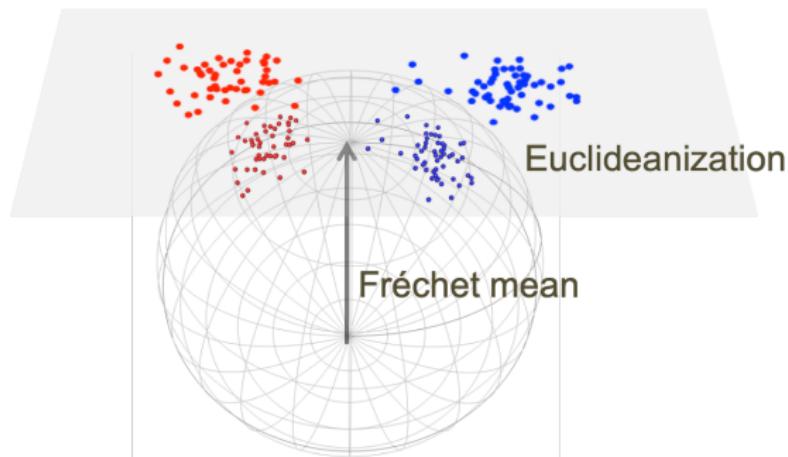
- Since each spoke direction is a unit vector, it lies on \mathbb{S}^2 . The problem of testing for a difference in spoke directions between the two groups can be visualized as follows:



An approach to test the difference

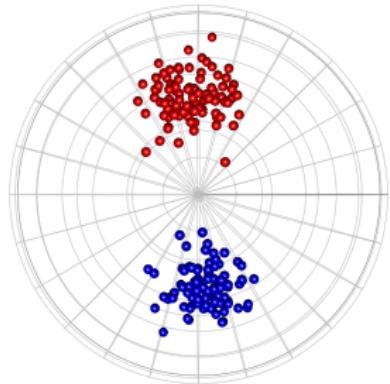
- (Tangent space) Calculate the Fréchet mean and consider the Tangent space at the Fréchet mean
- (Euclideanization) Map the data points to the tangent space at the Fréchet mean (via the logarithmic map).
- (Testing) Apply a standard Euclidean testing method, such as Hotelling's T^2 -test.

Tangent space at the Fréchet mean

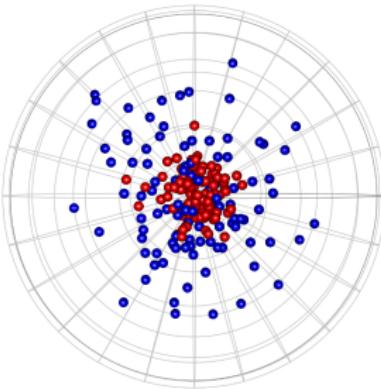


Research question

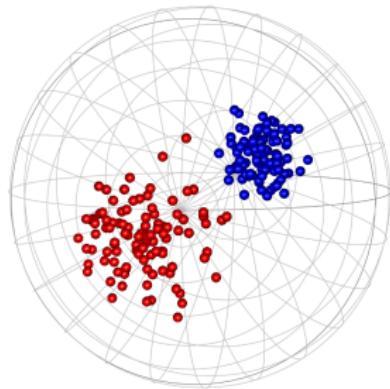
Location and/or dispersion problem



(a) Location



(b) Dispersion



(c) Both

- Existing regression models for a spherical response
 - Fisher & Lee (1992); Presnell et al. (1998): Limited to \mathbb{S}^1
 - Paine et al. (2020): No inferential procedure (potentially available)

Methods

von Mises-Fisher (vMF) distribution

- For $\mathbf{y} \in \mathbb{S}^{q-1}$, the probability density function of von Mises-Fisher distribution (vMF) is defined as

$$f_{vMF}(\mathbf{y} : \boldsymbol{\zeta}, \kappa) = C_q(\kappa) \exp\left(\kappa \boldsymbol{\zeta}^T \mathbf{y}\right)$$

for a concentration parameter $\kappa \geq 0$ and mean direction $\boldsymbol{\zeta} \in \mathbb{S}^{q-1}$.

- Here, $C_q(\kappa)$ is a normalization constant defined as

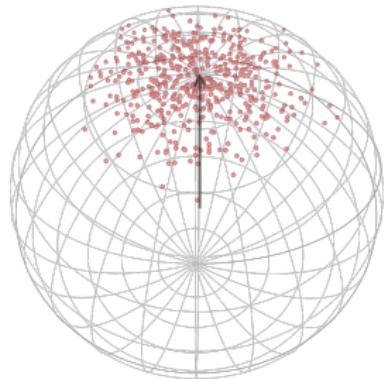
$$C_q(\kappa) = \frac{\kappa^{q/2-1}}{(2\pi)^{q/2} I_{q/2-1}(\kappa)},$$

where $I_\nu(\cdot)$ is the modified Bessel function of the first kind at order ν .

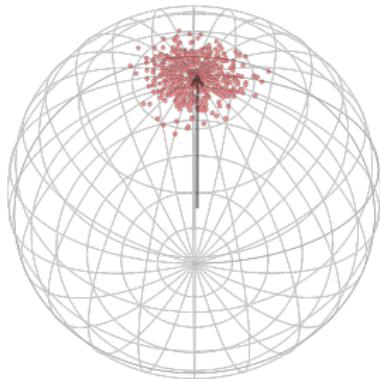
von Mises-Fisher (vMF) distribution

- An example of von Mises-Fisher distribution with

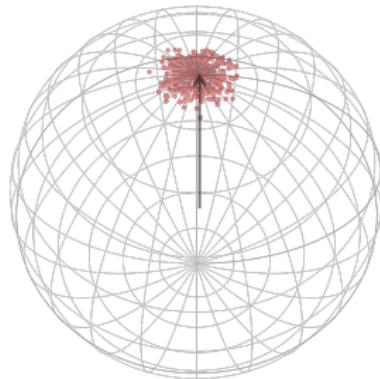
$$q = 3, \quad \zeta = (0, 0, 1)^\top, \quad \kappa \in \{5, 10, 15\}$$



(a) $\kappa = 5$



(b) $\kappa = 10$



(c) $\kappa = 15$

von Mises-Fisher (vMF) distribution

- Constraint on a mean direction parameter
 - A mean direction ζ of vMF belongs to \mathbb{S}^{q-1} , so it is not directly linked to a linear predictor $\boldsymbol{\eta}_i = \boldsymbol{\mu} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j \in \mathbb{R}^q$

$$\zeta_i \stackrel{?}{=} \boldsymbol{\mu} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j$$

for $\boldsymbol{\mu} \in \mathbb{R}^q$.

- A concentration parameter κ of vMF is also constrained

$$\kappa \in \mathbb{R}_+ := \{c \in \mathbb{R} : c \geq 0\}$$

- We want to link the mean direction to a linear predictor without constraints.

A double regression model for location and dispersion

- For a linear predictor η_i , we can consider two types of link functions:
 - Location link:

$$\zeta_i = \frac{\boldsymbol{\eta}_i^{\text{loc}}}{\|\boldsymbol{\eta}_i^{\text{loc}}\|_2} \Rightarrow g_1(\zeta_i) = \boldsymbol{\eta}_i^{\text{loc}} = \boldsymbol{\mu}^{\text{loc}} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j^{\text{loc}}$$

- Dispersion link:

$$\kappa_i = \|\boldsymbol{\eta}_i^{\text{disp}}\| \Rightarrow g_2(\kappa_i) = \boldsymbol{\eta}_i^{\text{disp}} = \boldsymbol{\mu}^{\text{disp}} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j^{\text{disp}}$$

- The log-likelihood can be written as

$$\begin{aligned}\ell(\boldsymbol{\mu}^{\text{loc}}, \boldsymbol{\mu}^{\text{disp}}, \mathbf{B}^{\text{loc}}, \mathbf{B}^{\text{disp}} | \mathbf{Y}) &= \sum_{i=1}^n \kappa_i \zeta_i^\top \mathbf{y}_i + \log C_q(\kappa_i) \\ &= \sum_{i=1}^n \|\boldsymbol{\eta}_i^{\text{disp}}\|_2 \frac{\boldsymbol{\eta}_i^{\text{loc}}^\top \mathbf{y}_i}{\|\boldsymbol{\eta}_i^{\text{loc}}\|_2} + \log C_q(\|\boldsymbol{\eta}_i^{\text{disp}}\|_2)\end{aligned}\tag{2}$$

A shared parameter model for location and dispersion

- Alternatively, we can consider the model with shared parameter β_j between location and dispersion link functions:
 - Location link:

$$\zeta_i = \frac{\boldsymbol{\eta}_i}{\|\boldsymbol{\eta}_i\|_2} \Rightarrow g_1(\zeta_i) = \boldsymbol{\eta}_i = \boldsymbol{\mu} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j$$

- Dispersion link:

$$\kappa_i = \|\boldsymbol{\eta}_i\| \Rightarrow g_2(\kappa_i) = \boldsymbol{\eta}_i = \boldsymbol{\mu} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j$$

- The log-likelihood can be written as

$$\begin{aligned}\ell(\boldsymbol{\mu}, \mathbf{B} | \mathbf{Y}) &= \sum_{i=1}^n \kappa_i \zeta_i^\top \mathbf{y}_i + \log C_q(\kappa_i) \\ &= \sum_{i=1}^n \boldsymbol{\eta}_i^\top \mathbf{y}_i + \log C_q(\|\boldsymbol{\eta}_i\|_2)\end{aligned}\tag{3}$$

Reparameterization

- The shared parameter model is equivalent to the model with **reparameterization** $\boldsymbol{\theta} = \kappa \cdot \boldsymbol{\zeta} \in \mathbb{R}^q$
- This leads to a reparameterized vMF distribution with a mean vector $\boldsymbol{\theta} \in \mathbb{R}^q$:

$$f_{\text{vMF}}(\mathbf{y} : \boldsymbol{\theta}) = \exp \left(\boldsymbol{\theta}^T \mathbf{y} + \log C_q(\|\boldsymbol{\theta}\|) \right). \quad (4)$$

- This reparameterization reveals that the vMF distribution is a member of the **canonical exponential family** with the natural parameter $\boldsymbol{\theta}$.
- More specifically, by comparing the canonical exponential family form

$$f(\mathbf{y} | \boldsymbol{\theta}, \phi) = \exp \left(\frac{\boldsymbol{\theta}^T \mathbf{y} - b(\boldsymbol{\theta})}{a(\phi)} + c(\mathbf{y}, \phi) \right),$$

it turns out that

$$a(\phi) = 1, \quad b(\boldsymbol{\theta}) = -\log C_q(\|\boldsymbol{\theta}\|), \quad \text{and} \quad c(\mathbf{y}, \phi) = 0$$

Proposition 1

For $\boldsymbol{\theta} \in \mathbb{R}^q$ with $\|\boldsymbol{\theta}\| \neq 0$, the first and second derivatives of $b(\boldsymbol{\theta})$ can be expressed as

$$b'(\boldsymbol{\theta}) = \frac{\boldsymbol{\theta}}{\|\boldsymbol{\theta}\|} \left\{ \frac{I_{q/2}(\|\boldsymbol{\theta}\|)}{I_{q/2-1}(\|\boldsymbol{\theta}\|)} \right\}$$

$$b''(\boldsymbol{\theta}) = \left(\frac{\boldsymbol{\theta}}{\|\boldsymbol{\theta}\|} \right) \left(\frac{\boldsymbol{\theta}}{\|\boldsymbol{\theta}\|} \right)^T H_q(\|\boldsymbol{\theta}\|) + \frac{B_q(\|\boldsymbol{\theta}\|)}{\|\boldsymbol{\theta}\|} \left\{ \mathbf{I} - \left(\frac{\boldsymbol{\theta}}{\|\boldsymbol{\theta}\|} \right) \left(\frac{\boldsymbol{\theta}}{\|\boldsymbol{\theta}\|} \right)^T \right\},$$

where $B_q(\kappa) = \frac{I_{q/2}(\kappa)}{I_{q/2-1}(\kappa)}$ is the ratio of the modified Bessel functions (also known as the Mean Resultant Length) and

$$H_q(\kappa) = 1 - B_q^2(\kappa) - \frac{q-1}{\kappa} B_q(\kappa)$$

Linking the spherical responses to covariates

- We can consider the generalized linear model for the reparametrized vMF distribution as

$$g(\mathbb{E}[\mathbf{y}_i | \mathbf{x}_i]) = \boldsymbol{\theta}_i = \boldsymbol{\mu} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j = \boldsymbol{\mu} + \mathbf{B}^T \mathbf{x}_i$$
$$\mathbf{y}_i | \mathbf{x}_i \sim \text{vMF}(\boldsymbol{\theta}_i),$$

where

- $\mathbf{y}_i \in \mathbb{S}^{q-1}$, $\boldsymbol{\mu}, \boldsymbol{\theta}_i \in \mathbb{R}^q$,
- $g(\xi) = B_q^{-1}(\|\xi\|) \frac{\xi}{\|\xi\|}$ is a known link function,
- $\mathbf{x}_i = (x_{i1}, \dots, x_{ip})^T$ is a p -dimensional covariate vector, and $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^T$ is a column-centered design matrix.
- $\mathbf{B} = [\mathbf{B}_1, \dots, \mathbf{B}_q] \in \mathbb{R}^{p \times q}$ is a coefficient matrix whose the (j, k) -th element represents the effect of j -th covariate on the k -th response.

■ Let us define

- $\tilde{\mathbf{x}}_i := \mathbf{x}_i \otimes \mathbf{I}_q \in \mathbb{R}^{pq \times q}$
- $\boldsymbol{\beta}^* := \text{vec}(\mathbf{B}^T) = (\boldsymbol{\beta}_1^T, \boldsymbol{\beta}_2^T, \dots, \boldsymbol{\beta}_p^T)^T \in \mathbb{R}^{pq \times 1}$

■ Then, we can write the model as

$$\boldsymbol{\theta}_i = \boldsymbol{\mu} + \tilde{\mathbf{x}}_i^T \boldsymbol{\beta}^*. \quad (5)$$

and its log-likelihood as

$$\ell(\boldsymbol{\mu}, \boldsymbol{\beta}^*) = \sum_{i=1}^n \left\{ \boldsymbol{\mu}^T \mathbf{y}_i + \boldsymbol{\beta}^{*T} \tilde{\mathbf{x}}_i \mathbf{y}_i - b(\boldsymbol{\mu} + \tilde{\mathbf{x}}_i^T \boldsymbol{\beta}^*) \right\}, \quad (6)$$

- Let us denote the full parameter vector by $\gamma = (\mu^\top, \beta^{*\top})^\top$.
- The corresponding score function $s_n(\gamma)$ and Fisher information matrix $\mathbf{F}_n(\gamma)$ are given by

Proposition 2

$$s_n(\gamma) = \frac{\partial \ell(\gamma)}{\partial \gamma} = \sum_{i=1}^n \tilde{x}_i \left\{ y_i - b'(\mu + \tilde{x}_i^T \beta^*) \right\}$$

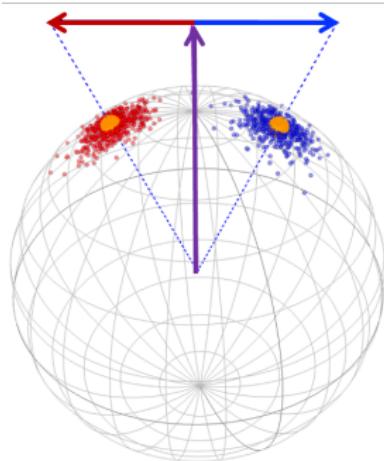
$$\mathbf{F}_n(\gamma) = \frac{\partial^2 \ell(\gamma)}{\partial \gamma \partial \gamma^T} = \sum_{i=1}^n \left\{ \tilde{x}_i b''(\mu + \tilde{x}_i^T \beta^*) \tilde{x}_i^T \right\}.$$

Proposition 3

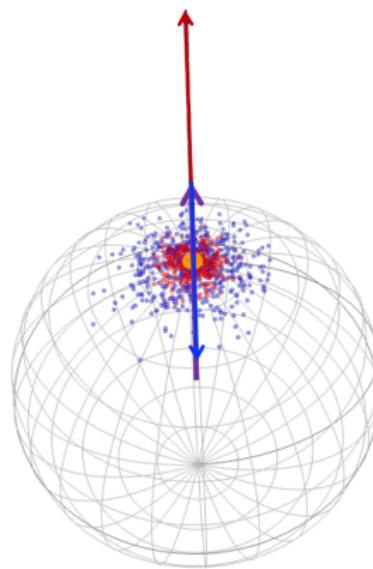
If $\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T$ is of full rank, the Fisher information matrix is positive definite, and the MLE of γ is unique

- Recall that

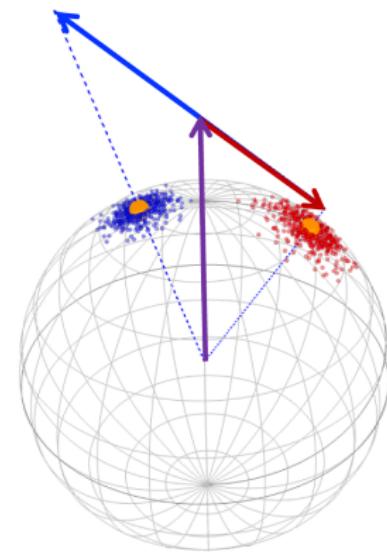
$$\boldsymbol{\theta}_i = \boldsymbol{\mu} + \sum_{j=1}^p x_{ij} \boldsymbol{\beta}_j \in \mathbb{R}^q, \quad \mathbf{y}_i | \mathbf{x}_i \sim \text{vMF}(\boldsymbol{\theta}_i) \text{ with } x_{ij} \in \{-1, +1\},$$



(a) orthogonal



(b) parallel



(c) oblique

Maximum likelihood estimation with or without constraints

- Unconstrained Maximum likelihood estimation (MLE):

$$\arg \max_{\boldsymbol{\mu} \in \mathbb{R}^q, \boldsymbol{\beta}^* \in \mathbb{R}^{pq}} \sum_{i=1}^n \left\{ (\boldsymbol{\mu} + \tilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}^*)^T \mathbf{y}_i + \log C_q(\|\boldsymbol{\mu} + \tilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}^*\|) \right\}$$

- Constrained MLE under orthogonality constraints:

$$\arg \max_{\boldsymbol{\mu} \in \mathbb{R}^q, \boldsymbol{\beta}^* \in \mathbb{R}^{pq}} \sum_{i=1}^n \left\{ (\boldsymbol{\mu} + \tilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}^*)^T \mathbf{y}_i + \log C_q(\|\boldsymbol{\mu} + \tilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}^*\|) \right\}$$

subject to $\boldsymbol{\beta}_j \perp \boldsymbol{\mu} \quad \forall j = 1, \dots, p$

- If the true parameters satisfy this constraint, the constrained estimator can be more efficient (i.e., have lower variance).

- Let us denote the constrained estimator of γ by $\hat{\gamma}^c$ and the unconstrained version by $\hat{\gamma}^{uc}$. Then, we have

Theorem 1

- Under the regularity conditions, the weak consistency and the asymptotic normality of $\hat{\gamma}^c$ can be obtained as follows:*

$$\hat{\gamma}^{uc} \xrightarrow{p} \gamma_0 \text{ and } \hat{\gamma}^{uc} \xrightarrow{d} N(\gamma_0, \mathbf{F}(\gamma_0)^{-1}).$$

- By further assuming that $\beta_{j,0} \perp \mu_0 \forall j$, we then have*

$$\hat{\gamma}^c \xrightarrow{p} \gamma_0 \text{ and } \hat{\gamma}^c \xrightarrow{d} N(\gamma_0, \Sigma_c),$$

where the asymptotic covariance matrix Σ_c is given by

$$\mathbf{F}(\gamma_0)^{-1} - \mathbf{F}(\gamma_0)^{-1} \mathbf{H}_0^\top \left(\mathbf{H}_0 \mathbf{F}(\gamma_0)^{-1} \mathbf{H}_0^\top \right)^{-1} \mathbf{H}_0 \mathbf{F}(\gamma_0)^{-1}$$

and $\mathbf{H}_0 = \mathbf{H}_0(\gamma_0)$ is the Jacobian of the constraints w.r.t. γ at γ_0 .

Corollary 2 (Asymptotic Normality via Projection)

Let us let $\mathbf{P}_{\hat{\boldsymbol{\mu}}} = \hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}^T/\|\hat{\boldsymbol{\mu}}\|^2$, $\mathbf{P}_{\hat{\boldsymbol{\mu}}^\perp} = \mathbf{I} - \mathbf{P}_{\hat{\boldsymbol{\mu}}}$ be the projection matrix onto $\hat{\boldsymbol{\mu}}$ and its orthogonal complement, respectively.

□ Under the regularity conditions, as $n \rightarrow \infty$, we have

$$\mathbf{P}_{\hat{\boldsymbol{\mu}}^\perp}\hat{\boldsymbol{\beta}}_j^{uc} | \hat{\boldsymbol{\mu}} \xrightarrow{d} N(\mathbf{P}_{\boldsymbol{\mu}^\perp}\boldsymbol{\beta}_j^{uc}, \Sigma_{\boldsymbol{\mu}^\perp})$$

where $\Sigma_{\boldsymbol{\mu}^\perp} = \mathbf{P}_{\boldsymbol{\mu}^\perp}\mathbf{c}_j^T \left[\mathbf{F}_{0,22}^{-1} - \mathbf{F}_{0,21}^{-1}\mathbf{F}_{0,11}\mathbf{F}_{0,12}^{-1} \right] \mathbf{c}_j \mathbf{P}_{\boldsymbol{\mu}^\perp}^T$ and \mathbf{c}_j is the index matrix extracting the components representing the j -th covariate.
□ Similarly, for the $\boldsymbol{\mu}$ -directional projection, we have the following result:

$$\mathbf{P}_{\hat{\boldsymbol{\mu}}}\hat{\boldsymbol{\beta}}_j^{uc} | \hat{\boldsymbol{\mu}} \xrightarrow{d} N(\mathbf{P}_{\boldsymbol{\mu}}\boldsymbol{\beta}_j, \Sigma_{\boldsymbol{\mu}})$$

where $\Sigma_{\boldsymbol{\mu}} = \mathbf{P}_{\boldsymbol{\mu}}\mathbf{c}_j^T \left[\mathbf{F}_{0,22}^{-1} - \mathbf{F}_{0,21}^{-1}\mathbf{F}_{0,11}\mathbf{F}_{0,12}^{-1} \right] \mathbf{c}_j \mathbf{P}_{\boldsymbol{\mu}}^T$.

Confidence region

- Confidence regions of the unconstrained MLE, projected version onto μ and its orthogonal complement.

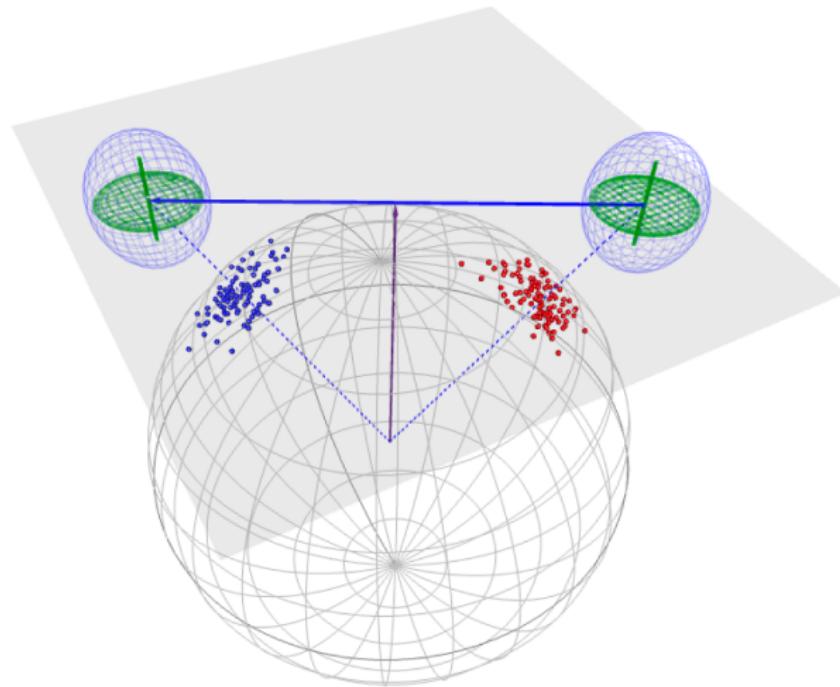


Figure: True coefficient vector $\beta_{0,1}$ is orthogonal to true mean vector μ_0

Simulation studies: two-sample test

- $n \in \{50, 100, 500, 1000\}$
- $q = 3$
- $\begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} \sim \mathcal{N} \left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right]$
 - $\rho \in \{0.2, 0.8\}$
- $X_1 = 2 \cdot \mathbb{1}(Z_1 \geq 0) - 1$
- $X_2 = Z_2$
- Data generating model:

$$\mathbf{y}_i \sim \text{vMF}(\boldsymbol{\theta}_i),$$

where $\boldsymbol{\theta}_i = \boldsymbol{\mu} + X_{i1}\boldsymbol{\beta}_1 + X_{i2}\boldsymbol{\beta}_2$ for $i = 1, \dots, n$.

Simulation studies: two-sample test

- $\mu = (0, 0, 20)^T$
- $\beta_j = \underbrace{\frac{\mathbf{d}_j}{\|\mathbf{d}_j\|_2}}_{\text{direction}} \times \underbrace{\mathcal{N}(0, s_j^2)}_{\text{length}}$ for $j = 1, 2$
 - Direction: $\mathbf{d}_j \in \text{span}(\mu)$ or $\mathbf{d}_j \in \text{span}(\mu)^\perp$,
 - $(\beta_1 \in \text{span}(\mu)^\perp, \beta_2 \in \text{span}(\mu)^\perp)$
 - $(\beta_1 \in \text{span}(\mu)^\perp, \beta_2 \in \text{span}(\mu))$
 - $(\beta_1 \in \text{span}(\mu), \beta_2 \in \text{span}(\mu)^\perp)$
 - $(\beta_1 \in \text{span}(\mu), \beta_2 \in \text{span}(\mu))$
 - Effect size: $s_j \in \{0, 2, 5\}$ for $j = 1, 2$
- The number of simulations = 100

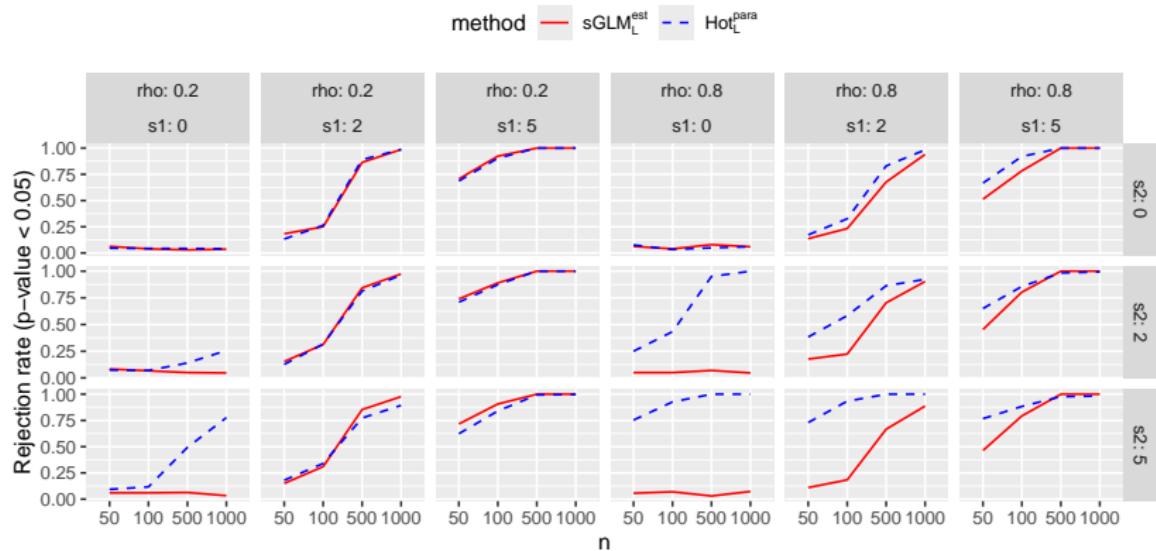
Comparing methods

- $s\text{GLM}_L^{\hat{\mu}^\perp}$: Location model of sphereGLM projected onto the orthogonal complement of the estimated $\hat{\mu}$
- $s\text{GLM}_D^{\hat{\mu}}$: Dispersion model of sphereGLM projected onto the estimated $\hat{\mu}$
- $\text{Hot}_L^{\text{para}}$: Hotelling's T^2 test
- $\text{Disp}_D^{\text{para}}$: Distance-based dispersion test¹

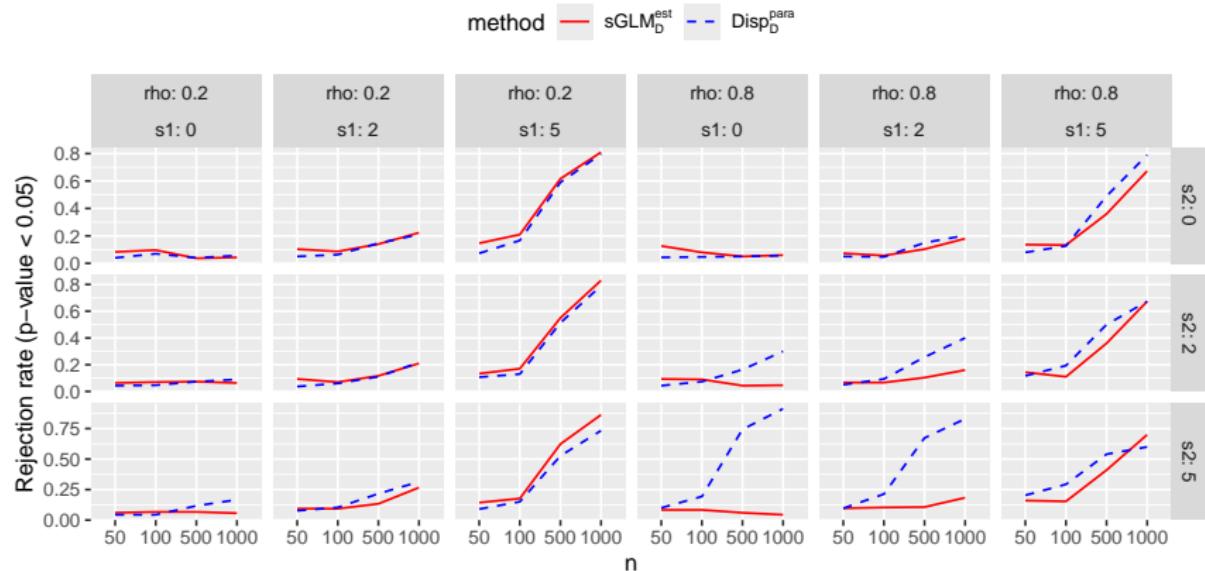
where # of perms = 5000

- Evaluation criteria
 - (i) Type I error rate and (ii) Statistical power

$$(\beta_1 \in \text{span}(\mu)^\perp, \beta_2 \in \text{span}(\mu)^\perp)$$

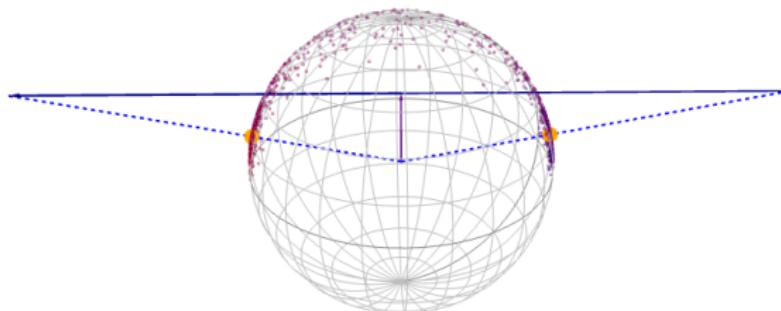


$$(\beta_1 \in \text{span}(\mu), \beta_2 \in \text{span}(\mu))$$



Concluding remarks

- A limitation arises with continuous covariates:
 - The domain of the conditional expectation $\mathbb{E}[y_i|x_i]$ may be restricted to a hemisphere. As a result, it would be difficult to account for spherical response



- As the parameter θ_i varies with the covariate, the location and dispersion effects become entangled. Disentangling these two effects remains a task for future work.
- Future work includes extending the model to multivariate responses on product manifolds, such as the torus ($\mathbb{S}^1 \times \mathbb{S}^1$), products of spheres ($\mathbb{S}^2 \times \mathbb{S}^2$), or a cylinder ($\mathbb{S}^2 \times \mathbb{R}_+$).

Thank you for your attention !

