

# Model-based Assessment of Functional and Phylogenetic Diversity



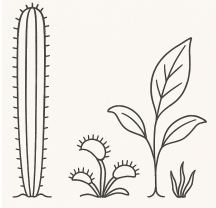

Shaoqian Huang

Supervisor: Prof. David Warton  
School of Mathematics and Statistics  
University of New South Wales

27 November 2025

1. An Introduction of Basic Concepts
2. From Distance-based Measures to Model-based Assessment
3. Model-based Assessment of PD and FD
4. The Future Work

# Phylogenetic Diversity (PD) vs Functional Diversity (FD)

Definition	High Diversity	Low Diversity
<b>PD</b> The extent to which species differ in their <b>evolutionary history</b> .	 Fig. 1	 Fig. 2
<b>FD</b> The extent to which species differ in their <b>functional traits</b> .	 Fig. 3	 Fig. 4

# Rao's Quadratic Entropy (Rao's Q)

$$Q = \mathbf{p}^\top \mathbf{D} \mathbf{p} \quad (1)$$

- **D**: distance matrix, elements  $d_{ij}$  = pairwise evolutionary/functional distances
- **p**: vector of relative abundances,  $\sum_i p_i = 1$

$$Q = \sum_i \sum_j p_i p_j d_{ij} \quad (2)$$

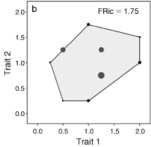
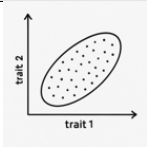
- **A mean dissimilarity measure.**

# Distance-based Measures for PD/FD

Sub-category	Method	Formula	PD?	FD?
Mean dissimilarity	Rao's Q	$Q = \sum_i \sum_j p_i p_j d_{ij}$	Yes	Yes
	MPD	$MPD = \frac{\sum_{i < j} d_{ij}}{\binom{m}{2}}$	Yes	Yes
	FDis	$FDis = \frac{\sum_i p_i  x_i - \bar{x} }{\sum_i p_i}$	No	Yes
Dendrogram	Faith's PD	Faith's PD = $\sum$ branch lengths	Yes	Yes

References: Botta-Dukát (2005), Webb et al. (2002), Laliberté and Legendre (2010), Faith (1992), Petchey and Gaston (2002).

# Multivariate Space - based Measures for PD/FD

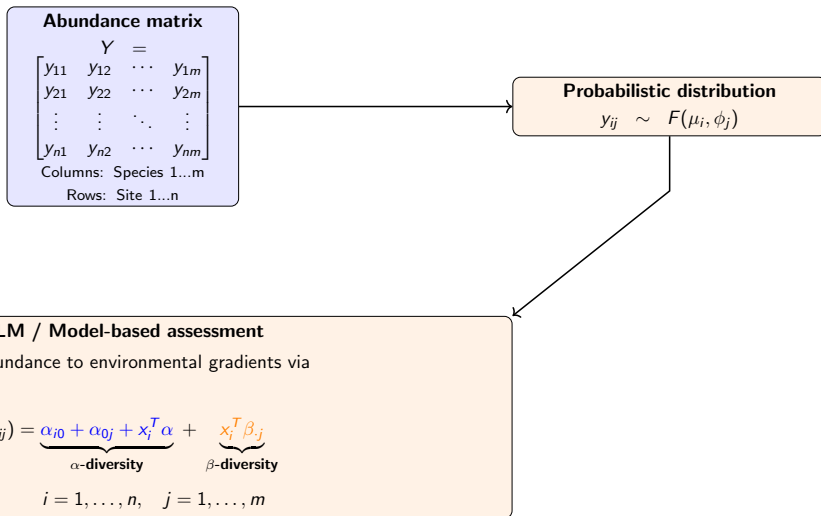
Method	Representation	PD?	FD?
Binary hypervolume		No	Yes
Probabilistic hypervolume		No	Yes

References: Villéger et al. (2008), Cornwell et al. (2006), Blonder (2016).

# From Distance-based Measures to Model-based Assessment

- Traditional measure (e.g. Rao's Q): mean dissimilarity.
  - Hard to evaluate how diversity changes along environmental gradients.
  - Highly sensitive to sampling intensity (i.e., how much effort is invested in data collection at each site).
- Model-based assessment (e.g. GLM):
  - Estimate compositional changes along environmental gradients.
  - Analyze their consequences for diversity changes.

# Model Abundance



*How to measure changes in PD/FD along gradients?*



## 1. Rao's Diversity Change

$$\Delta \text{Div}_{\text{Rao}} = |p_2^T D p_2 - p_1^T D p_1| = |p_2^T S p_2 - p_1^T S p_1|,$$

where  $D$  is a distance matrix and  $S > 0$  is a similarity matrix.

# A New Diversity Change Measure

## 1. Rao's Diversity Change

$$\Delta \text{Div}_{\text{Rao}} = |p_2^T D p_2 - p_1^T D p_1| = |p_2^T S p_2 - p_1^T S p_1|,$$

where  $D$  is a distance matrix and  $S > 0$  is a similarity matrix.

## 2. The Proposed Diversity Change

Let the relative abundance change be

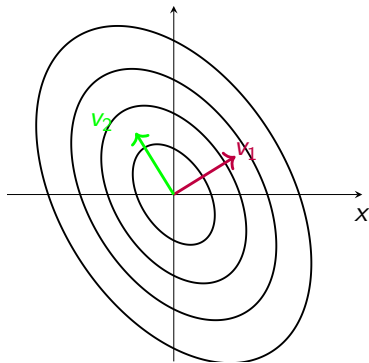
$$\beta = p_2 - p_1, \quad \sum_i \beta_i = 0.$$

The resulting diversity change is

$$\Delta \text{Div}_{\text{Model}} = \beta^T S \beta.$$

# Why the leading eigenvectors matter

Fig. 5: Contour of  $\beta^T S \beta$



## The main idea

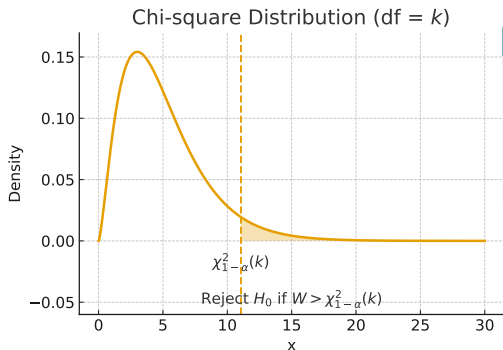
- If  $\beta \parallel v_1$ , PD/FD change.
- If  $\beta \perp v_1$ , No PD/FD change.

# Hypothesis Testing for PD/FD Change

## Hypothesis

$$H_0 : \text{No PD/FD change} \Leftrightarrow V_k^T \beta = \mathbf{0}.$$

Here,  $V_k = (\mathbf{v}_1, \dots, \mathbf{v}_k)$  is formed by the first  $k$  leading eigenvectors.



## Wald Test Statistic

$$W = (V_k^T \hat{\beta})^T [\text{Var}(V_k^T \hat{\beta})]^{-1} (V_k^T \hat{\beta}),$$

which follows a  $\chi^2$  distribution with  $k$  degrees of freedom under  $H_0$ .

$$p = 1 - F_{\chi_k^2}(W).$$

## Potential Rules for Determining $k$

$$V_k = (\mathbf{v}_1, \dots, \mathbf{v}_k)$$

denotes the matrix composed of the first  $k$  leading eigenvectors of  $S$ , corresponding to the eigenvalues  $\lambda_1, \dots, \lambda_k$ .

### Ways to determine $k$ :

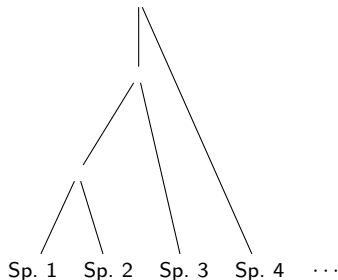
1. Pre-specify  $k$  (e.g.,  $k = 1$  or  $k = 2$ ).
2. Choose  $k$  such that the proportion of variance explained exceeds a threshold  $\tau$  (Proportion bigger than  $\tau$ ):

$$\frac{\sum_{i=1}^k \lambda_i}{\sum_{i=1}^m \lambda_i} \geq \tau.$$

3. Select  $k$  such that  $\lambda_i$  is greater than the mean eigenvalue (Bigger than averaged eigenvalues.):

$$\lambda_i > \frac{1}{m} \sum_{j=1}^m \lambda_j.$$

# Simulation Design



$$y_{ijh} \sim \text{Binomial}(1, \mu_{ij}), \quad \mu_{ij} = \text{expit}(x)$$

We vary sample size  $r$ ,  
# species  $m$ ,  
and # mean swaps  $s$ .

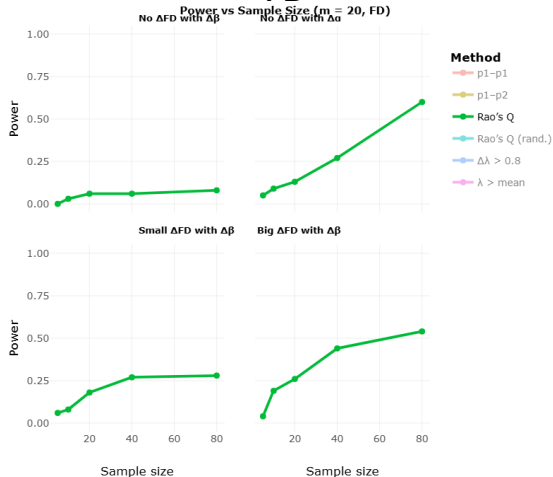
$$\text{Power} = \frac{\#\{\text{simulation with } p\text{-value} < 0.05\}}{\#\text{simulations}}$$

	Sp. 1	Sp. 2	Sp. 3	Sp. 4	...	Sp. $m$	$\Delta\beta$	$\Delta\alpha$	$\Delta\text{PD}/\Delta\text{FD}$
Com 1	$\text{expit}(-\beta)$	$\text{expit}(\beta)$	$\text{expit}(-\beta)$	$\text{expit}(\beta)$	...	$\text{expit}(\pm\beta)$		Reference	
Com 2	$\text{expit}(\beta)$	$\text{expit}(-\beta)$	$\text{expit}(-\beta)$	$\text{expit}(\beta)$	...	$\text{expit}(\pm\beta)$	$4\beta \cdot s$	No	No
Com 3	$\text{expit}(-\beta)$	$\text{expit}(-\beta)$	$\text{expit}(\beta)$	$\text{expit}(\beta)$	...	$\text{expit}(\pm\beta)$	$4\beta \cdot s$	No	Small
Com 4	$\text{expit}(\beta)$	$\text{expit}(\beta)$	$\text{expit}(-\beta)$	$\text{expit}(-\beta)$	...	$\text{expit}(\pm\beta)$	$4\beta \cdot s$	No	Big
Com 5	$\text{expit}(\alpha-\beta)$	$\text{expit}(\alpha+\beta)$	$\text{expit}(\alpha-\beta)$	$\text{expit}(\alpha+\beta)$	...	$\text{expit}(\alpha\pm\beta)$	No	$\alpha \cdot m$	No

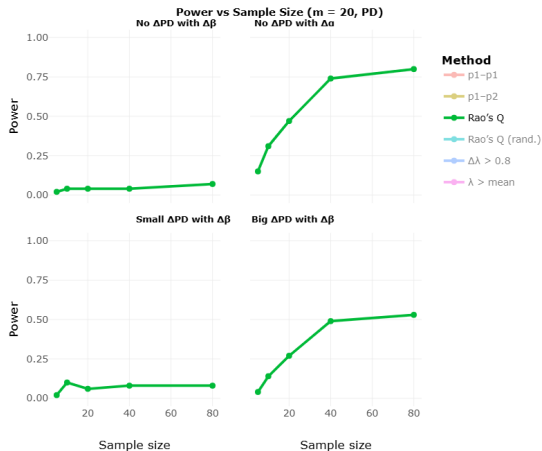
Note:  $\text{expit}(x) = \frac{e^x}{1+e^x}$ ;  $s = \#$  mean swaps; Com = community; Sp = species.

# Simulation Results

## FD



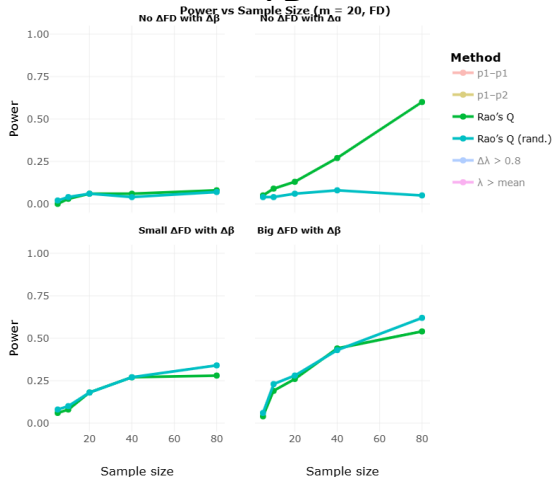
## PD



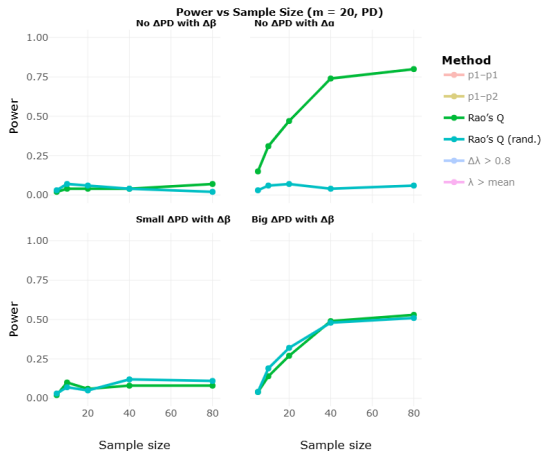
Rao's Q

# Simulation Results

## FD



## PD

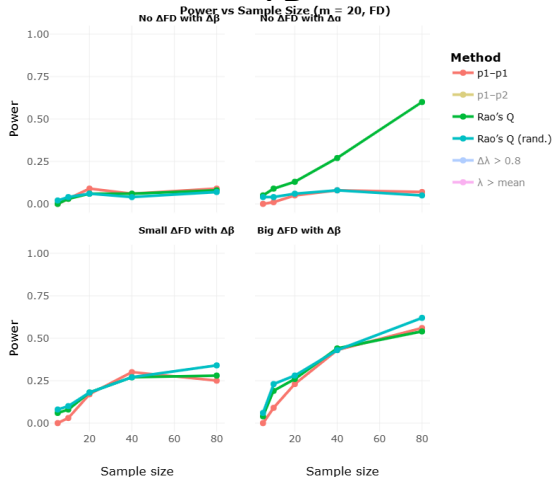


Rao's Q  $\rightarrow$  Rao's Q (rand.)

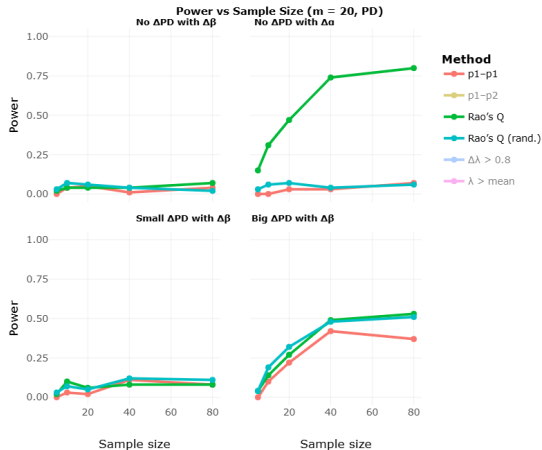


# Simulation Results

## FD



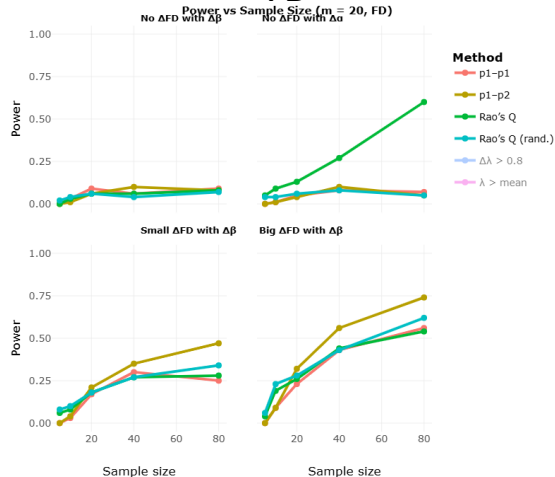
## PD



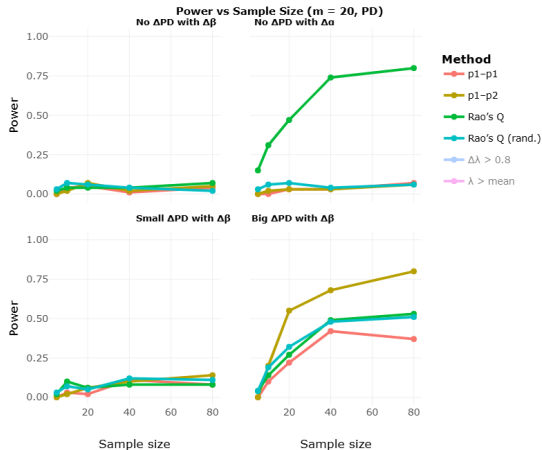
Rao's Q  $\rightarrow$  Rao's Q (rand.)  $\rightarrow$  **p1**

# Simulation Results

## FD



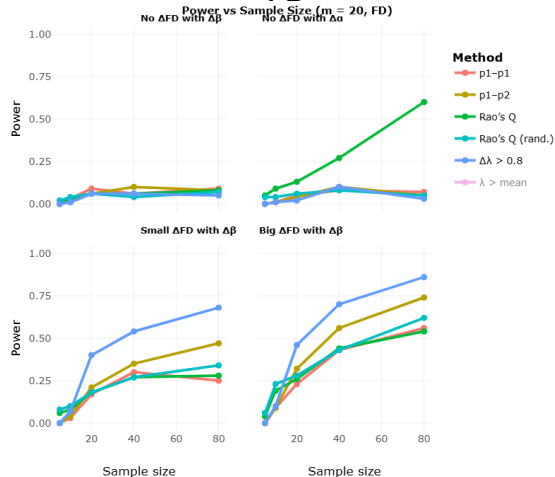
## PD



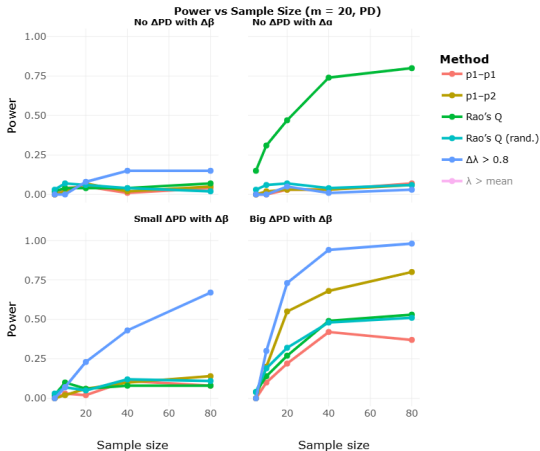
Rao's Q  $\rightarrow$  Rao's Q (rand.)  $\rightarrow$  p1  $\rightarrow$  p1,p2

# Simulation Results

## FD



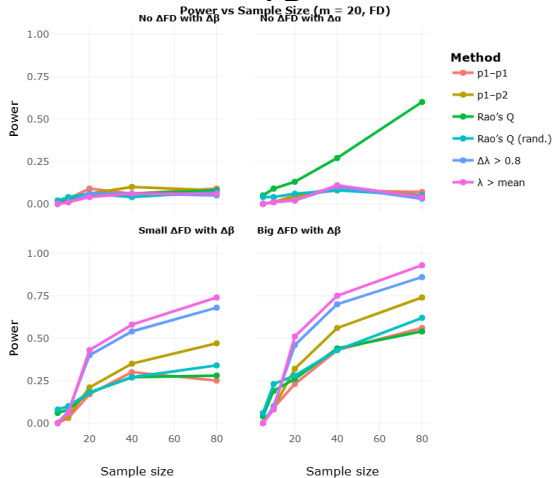
## PD



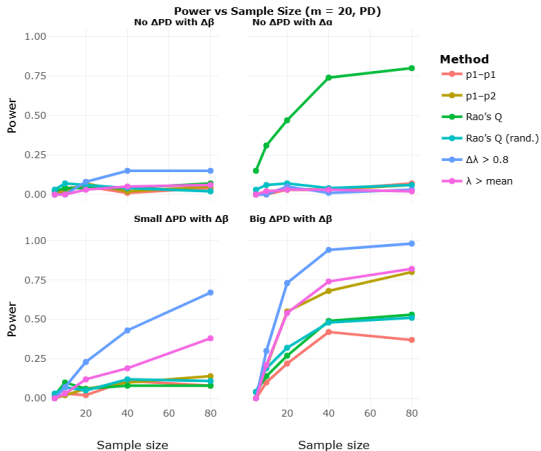
Rao's Q  $\rightarrow$  Rao's Q (rand.)  $\rightarrow p1 \rightarrow p1,p2 \rightarrow \Delta\lambda > 0.8$

# Simulation Results

## FD



## PD



Rao's Q  $\rightarrow$  Rao's Q (rand.)  $\rightarrow$  p1  $\rightarrow$  p1,p2  $\rightarrow$   $\Delta\lambda > 0.8$   $\rightarrow$   $\lambda > \text{mean}$

# The Future Work

- Implement large-scale simulations, including correlations between abundances and different distributions (e.g., Beta, Poisson)
- Apply the model to real-world case studies
- Develop a user-friendly software tool for FD and PD calculation

# References

- Blonder, B. (2016). Do hypervolumes have holes? *The American Naturalist*, 187(4):E93–E105. PMID: 27028084.
- Botta-Dukát, Z. (2005). Rao's quadratic entropy as a measure of functional diversity based on multiple traits. *Journal of Vegetation Science*, 16(5):533–540.
- Cornwell, W. K., Schwilk, D. W., and Ackerly, D. D. (2006). A trait-based test for habitat filtering: Convex hull volume. *Ecology*, 87(6):1465–1471.
- Faith, D. P. (1992). Conservation evaluation and phylogenetic diversity. *Biological Conservation*, 61(1):1–10.
- Laliberté, E. and Legendre, P. (2010). A distance-based framework for measuring functional diversity from multiple traits. *Ecology*, 91(1):299–305.
- Petchey, O. L. and Gaston, K. J. (2002). Functional diversity (fd), species richness and community composition. *Ecology Letters*, 5(3):402–411.
- Villéger, S., Mason, N. W. H., and Mouillot, D. (2008). New multidimensional functional diversity indices for a multifaceted framework in functional ecology. *Ecology*, 89(8):2290–2301.
- Webb, C. O., Ackerly, D. D., McPeck, M. A., and Donoghue, M. J. (2002). Phylogenies and community ecology. *Annual Review of Ecology, Evolution, and Systematics*, 33(Volume 33, 2002):475–505.

# The End