

# Model-based Assessment of Functional and Phylogenetic Diversity

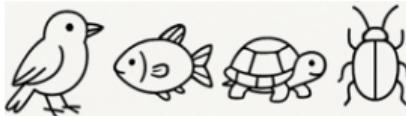
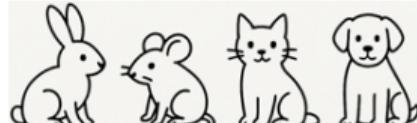
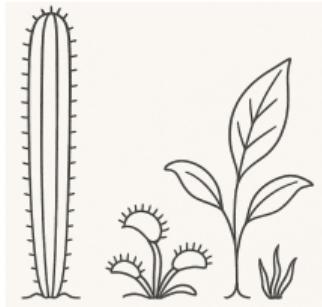
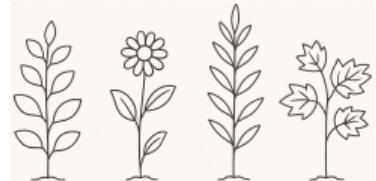
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1. An Introduction of Basic Concepts
2. From Distance-based Measures to Model-based Assessment
3. Model-based Assessment of PD and FD
4. The Future Work

# 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)

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

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

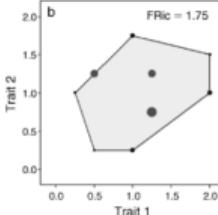
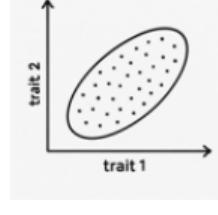
- $\mathbf{D}$ : distance matrix, elements  $d_{ij}$  = pairwise evolutionary/functional distances
- $\mathbf{p}$ : vector of relative abundances,  $\sum_i p_i = 1$
- A mean dissimilarity measure.

# 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	$\text{MPD} = \frac{\sum_{i < j} d_{ij}}{\binom{m}{2}}$	Yes	Yes
	FDis	$\text{FDis} = \frac{\sum_i p_i  x_i - \bar{x} }{\sum_i p_i}$	No	Yes
Dendrogram	Faith's PD	$\text{Faith's PD} = \sum \text{branch lengths}$	Yes	Yes

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

# Multivariate Space - based Measures for PD/FD

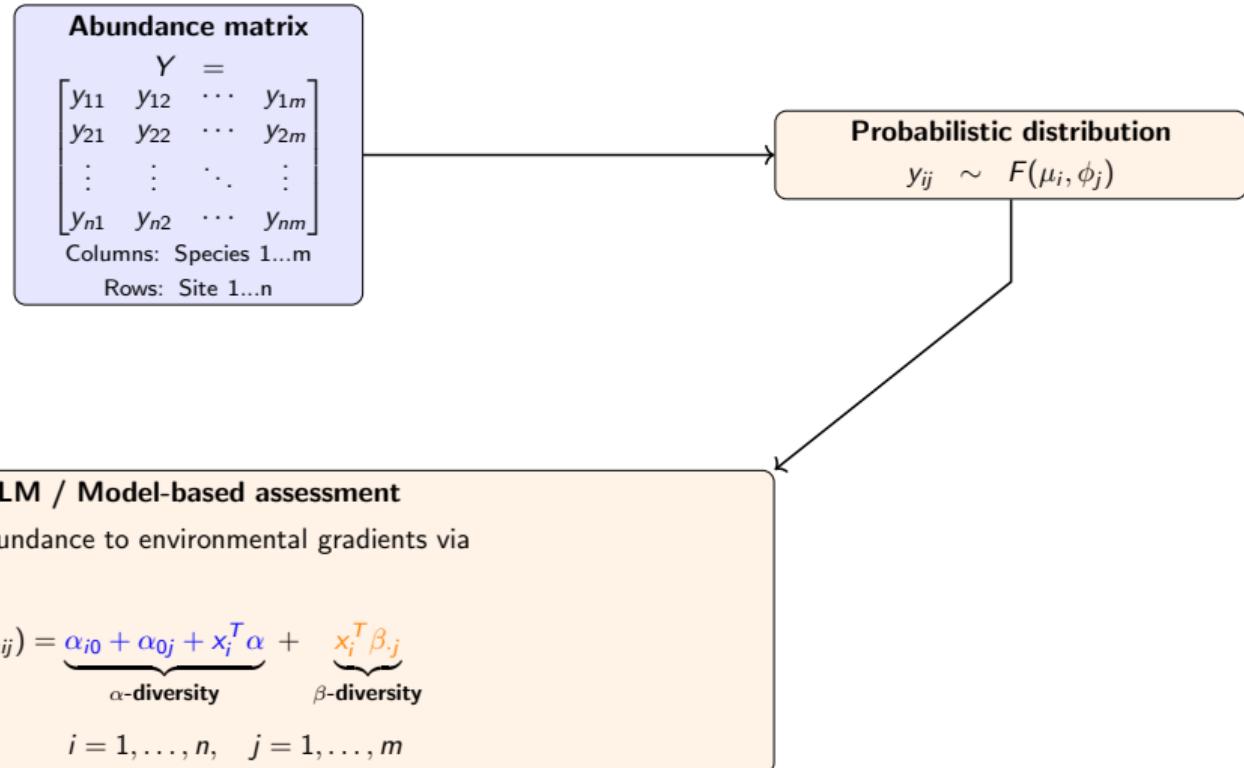
Method	Representation	PD?	FD?
Binary hypervolume		No	Yes
Probabilistic hypervolume		No	Yes

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

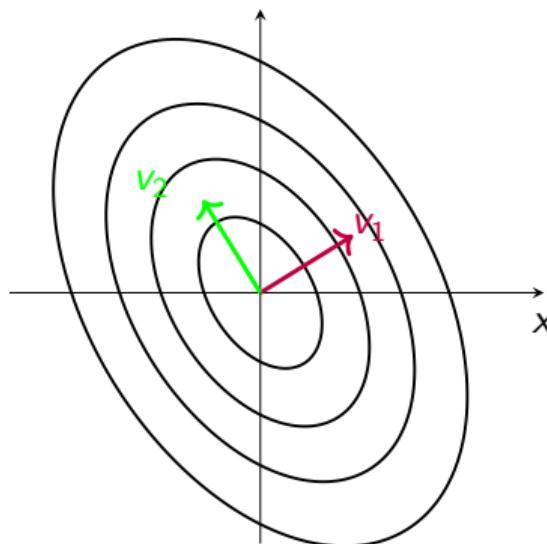
$$\beta = p_2 - p_1, \quad \sum_i \beta_i = 0.$$

The resulting diversity change is

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

# Why the leading eigenvectors matter

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



## The main idea

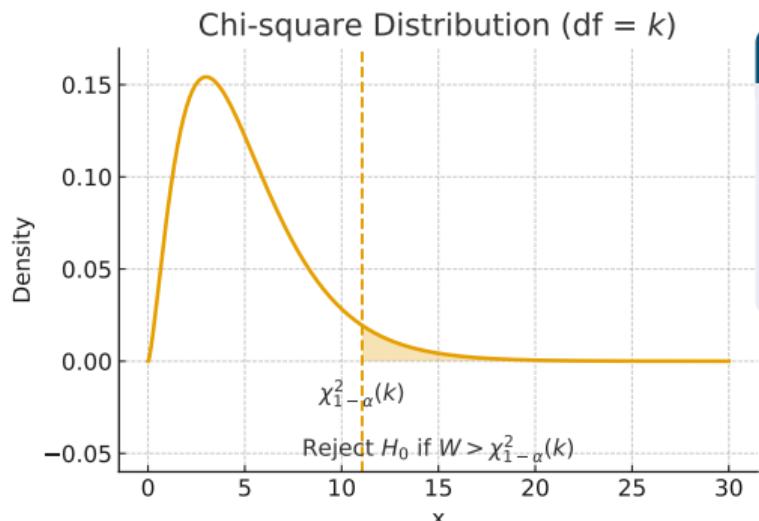
- If  $\beta \parallel v_1$ , PD/FD change.
- If  $\beta \perp v_1$ , No PD/FD change.

# 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

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

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 $k$ :

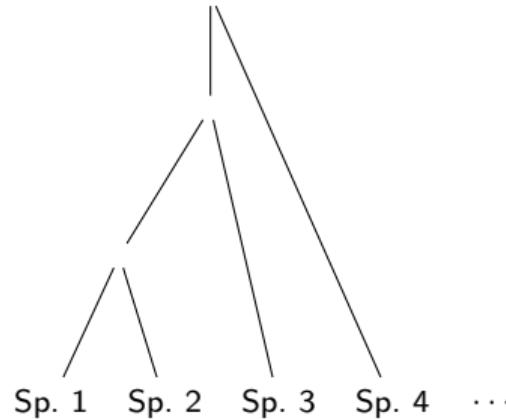
1. Pre-specify  $k$  (e.g.,  $k = 1$  or  $k = 2$ ).
2. Choose  $k$  such that the proportion of variance explained exceeds a threshold  $\tau$  (Proportion bigger than  $\tau$ .):

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

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



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

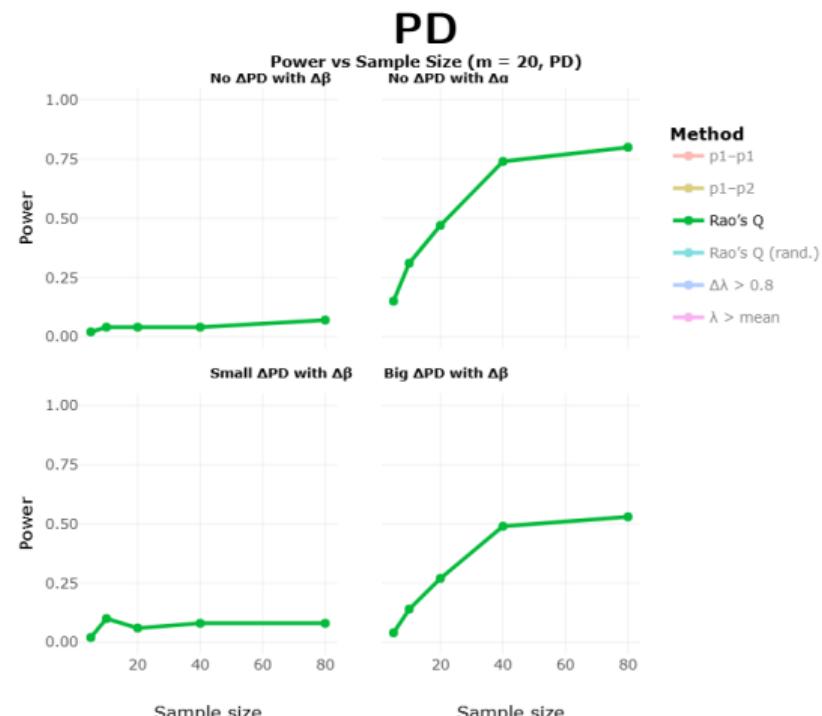
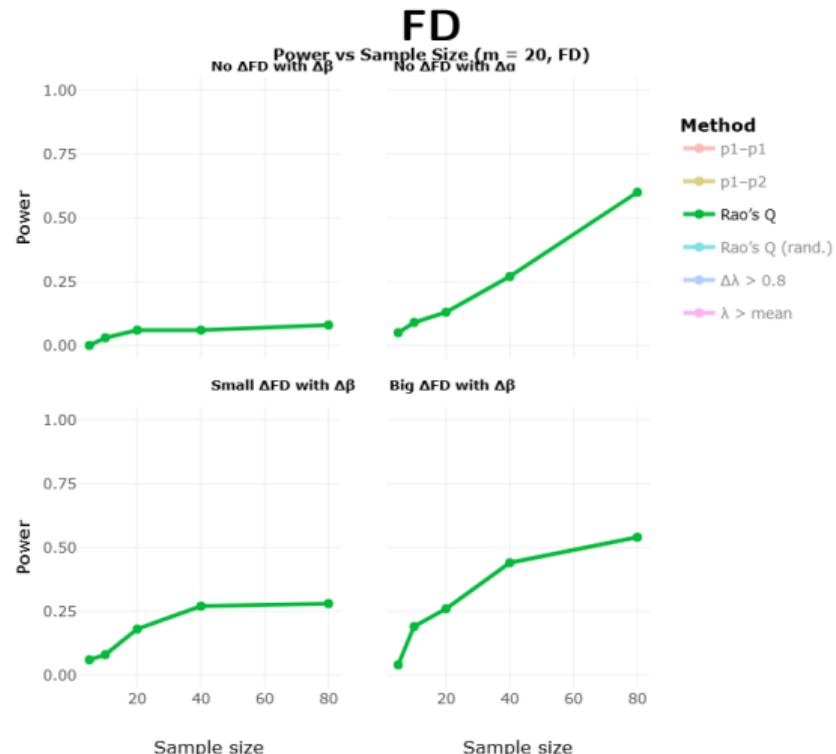
We vary sample size  $r$ ,  
# species  $m$ ,  
and # mean swaps  $s$ .

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

	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

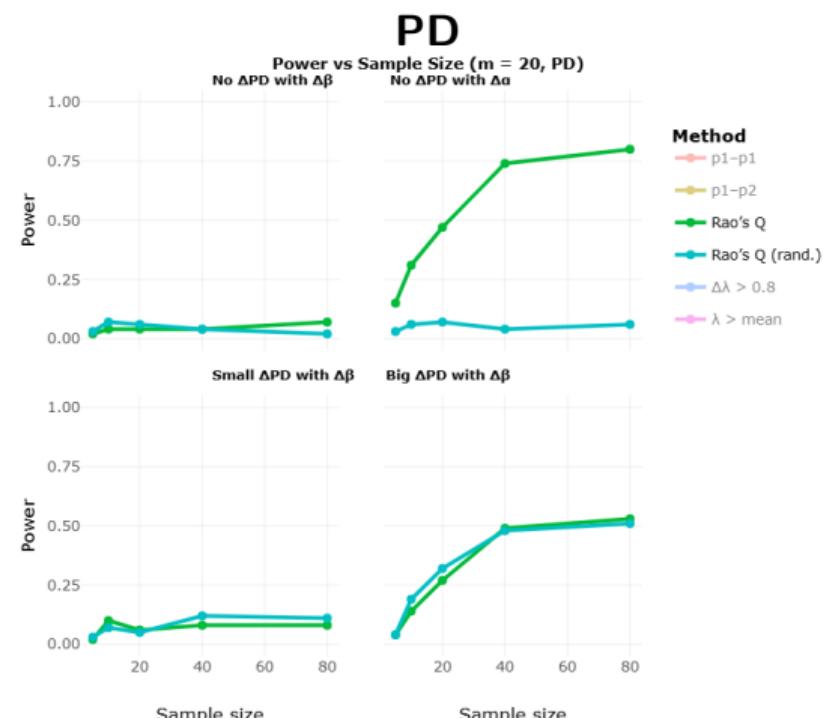
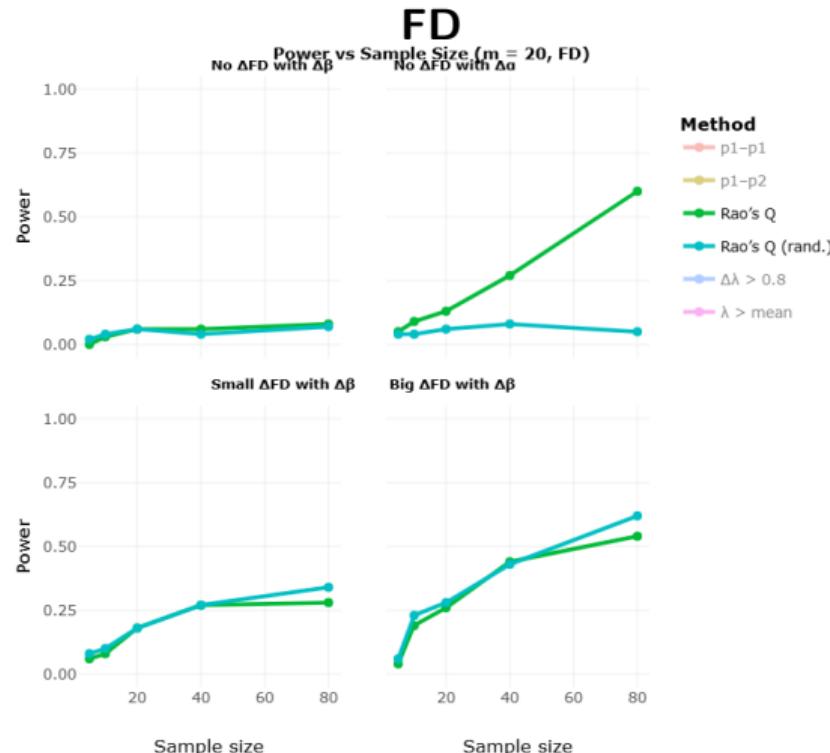
Note:  $\text{expit}(x) = \frac{e^x}{1+e^x}$ ;  $s = \# \text{ mean swaps}$ ; Com = community; Sp = species.

# Simulation Results



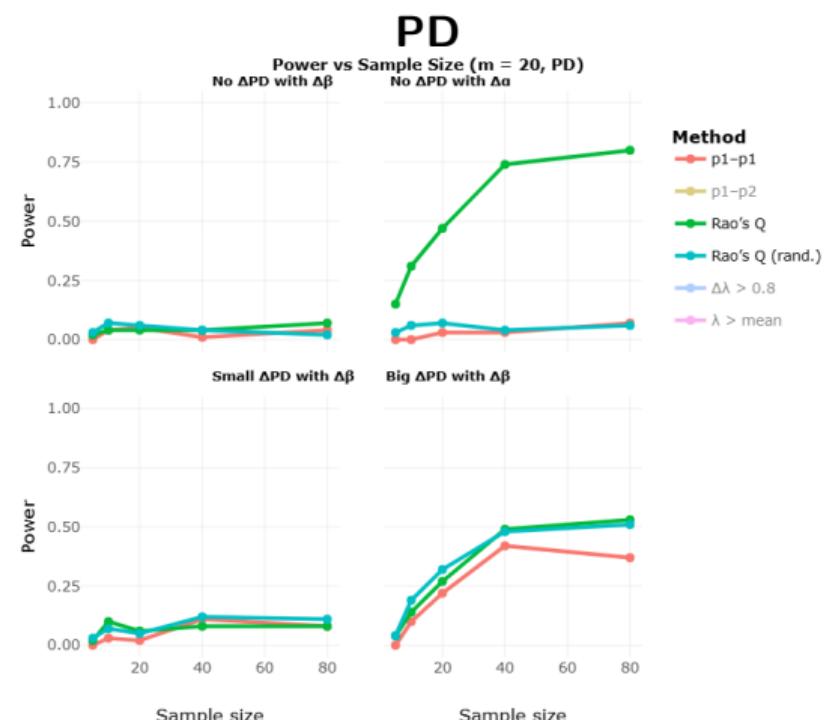
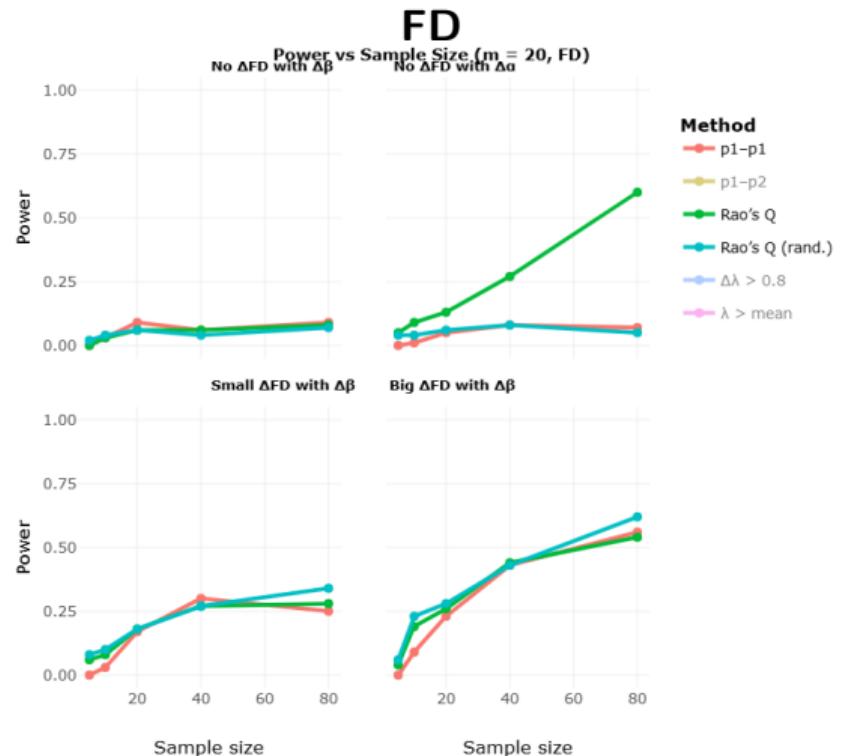
Rao's Q

# Simulation Results



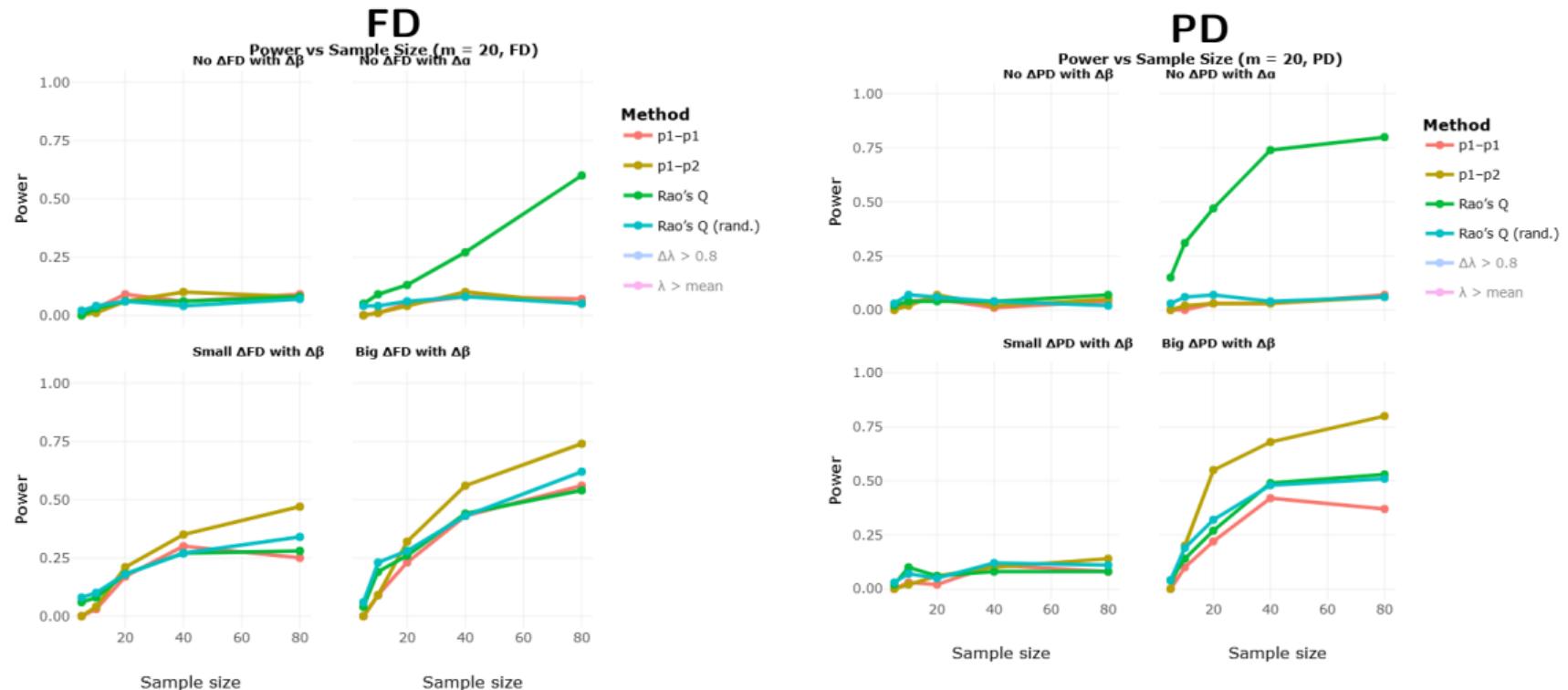
Rao's Q → Rao's Q (rand.)

# Simulation Results



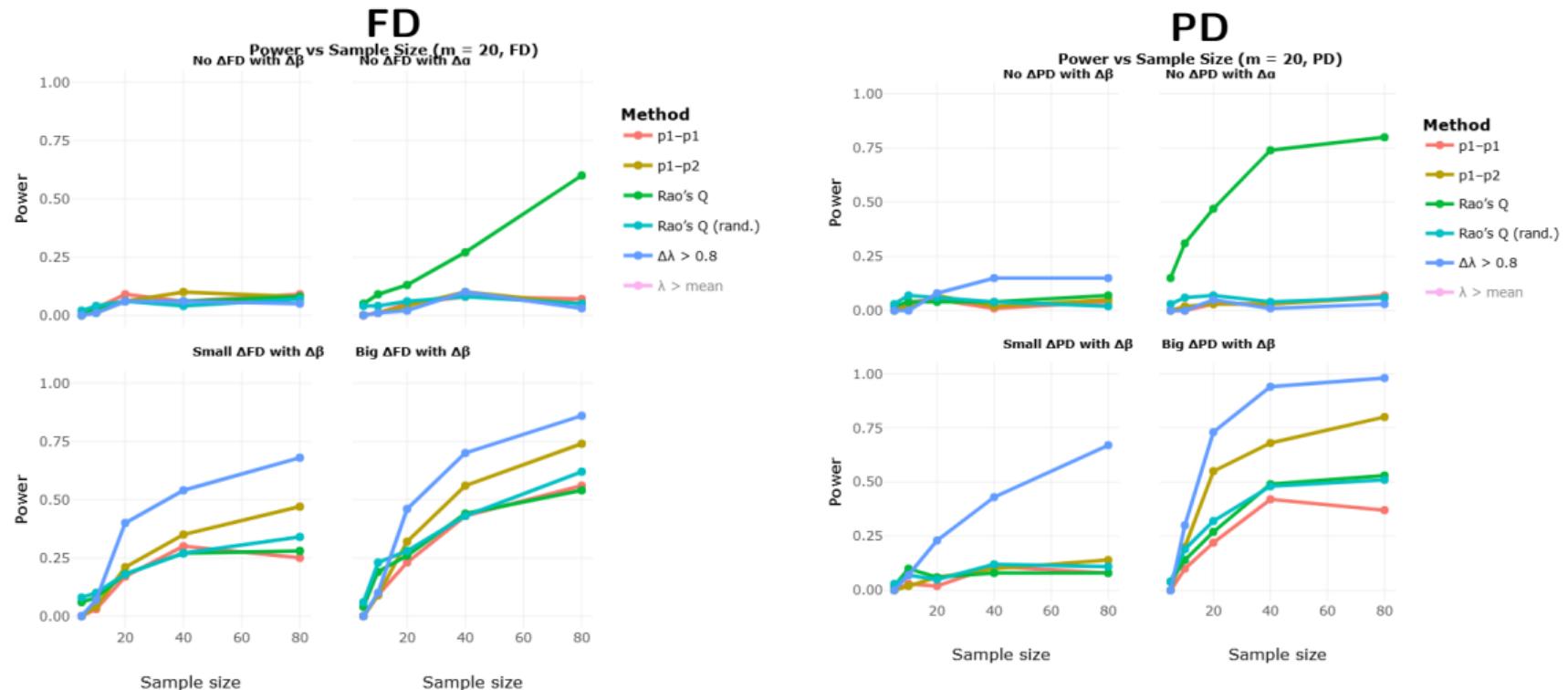
Rao's Q → Rao's Q (rand.) → p1

# Simulation Results



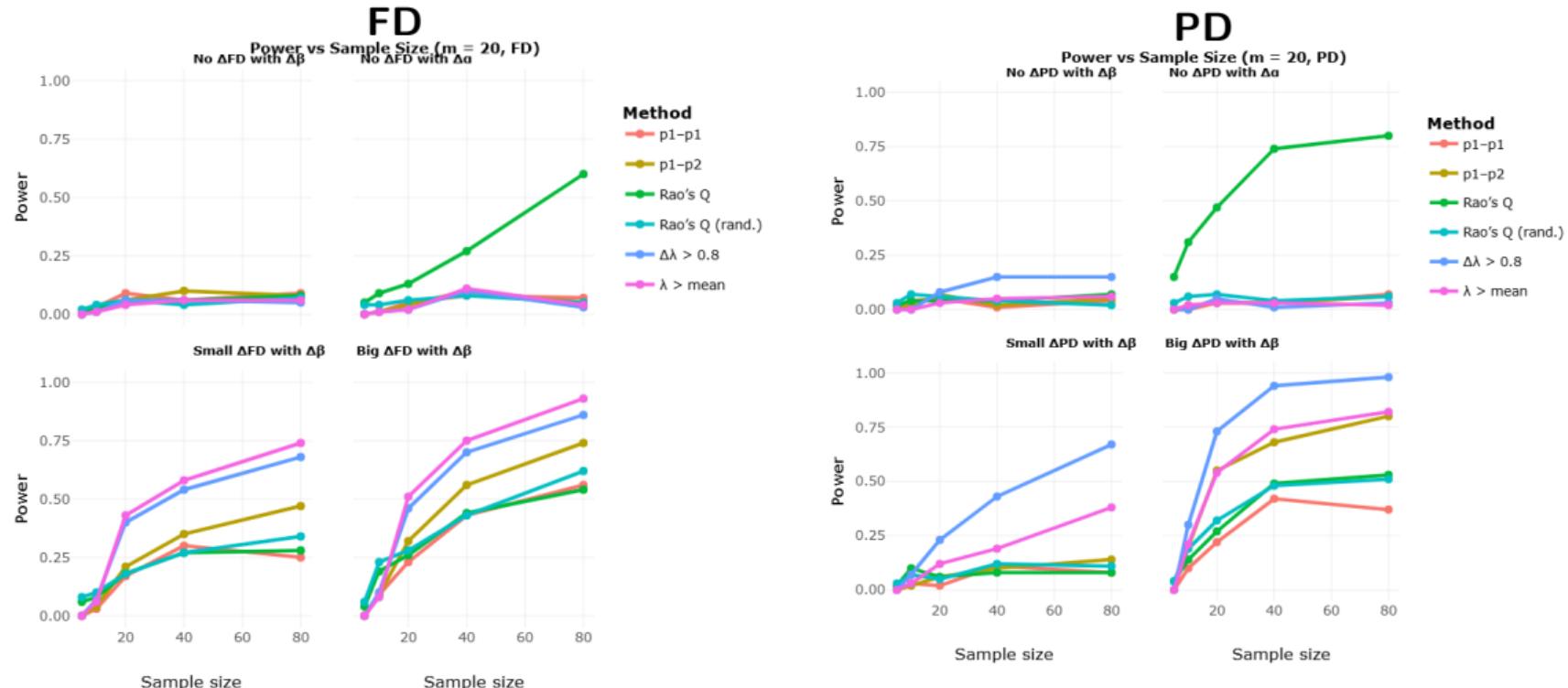
Rao's Q → Rao's Q (rand.) → p1 → p1,p2

# Simulation Results



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

# Simulation Results



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

## 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

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