Nonparametric MANOVA via Independence Testing

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Motivation

- Understand the relationship between k groups (*i.e.* control vs. disease)
- Question: Are they related? How?

One often desires to test groups

$\boldsymbol{U}$	$\boldsymbol{V}$
my grass	neighbor’s grass
human brain connectivity	alien brain connectivity
control	disease
cancer risk group 1	cancer risk group 2

One often desires to test groups

$\boldsymbol{U}$	$\boldsymbol{V}$
my grass	neighbor’s grass
human brain connectivity	alien brain connectivity
control	disease
cancer risk group 1	cancer risk group 2
any group	any other group

Statistics Background

- X is a random variable (some measurement)
- F_X is the distribution of X
- This means $F_X(a) = P(X \leq a)$
- This is denoted:

$$X \sim F_X$$

Statistics Background

- For two random variables X and Y, F_{XY} is called the joint distribution
- This means $F_{XY}(a, b) = P(X \leq a \text{ and } Y \leq b)$

  or,

$$(X, Y) \sim F_{XY}$$

Informal Definition of Hypothesis Testing

- **Null Hypothesis**: The conventional belief about a phenomenon of interest, written H_0.
- **Alternative Hypothesis**: An alternate belief about the same phenomenon, written H_A.
- **p-value**: The probability (under the null) of measurements more extreme than what was observed.

Formal Definition of *K*-Sample Testing

$$U_i^j \sim F_j, \qquad j \in 1, \ldots, k, \qquad i \in 1, \ldots, n_j$$

$$H_0 : F_1 = F_2 = \cdots = F_k$$

$$H_A : \exists\, j \neq j' \; s.t. \; F_j \neq F_{j'}$$

Note: These ideas and notation generalize for multivariate X and Y.

Outline

1. Intuition
2. Simulations
3. Multiway and Multilevel
4. Real Data
5. Conclusion

Intuition

Intuitive Desiderata of Testing Procedure

- Performant under *any* distribution
  - low- and high-dimensional
  - Euclidean and structured data (eg, sequences, images, networks, shapes)
  - linear and nonlinear relationships
- Is computational efficient

Provides a tractable algorithm that addresses the motivating question:

Are they related?

Analysis of Variance (ANOVA)

$$MST = \frac{\sum_{i=1}^{k} \left(T_i^2 / n_i \right) - G^2 / n}{k - 1}$$

$$MSE = \frac{\sum_{i=1}^{k} \sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^{k} \left(T_i^2 / n_i \right)}{n - k}$$

$$ANOVA = \frac{MST}{MSE}$$

Multivariate ANOVA (MANOVA)

$$\mathbf{W} = \sum_{i=1}^{k} \sum_{j=1}^{n_i} (\mathbf{x}_{ij} - \bar{\mathbf{x}}_{i\cdot})(\mathbf{x}_{ij} - \bar{\mathbf{x}}_{i\cdot})^T$$

$$\mathbf{B} = \sum_{i=1}^{k} n_i (\bar{\mathbf{x}}_{i\cdot} - \bar{\mathbf{x}}_{\cdot\cdot})(\bar{\mathbf{x}}_{i\cdot} - \bar{\mathbf{x}}_{\cdot\cdot})^T$$

$$MANOVA = \sum_{i=1}^{s} \frac{\lambda_i}{1 + \lambda_i} = \mathrm{tr}\left(\mathbf{B}(\mathbf{B} + \mathbf{W})^{-1}\right)$$

MANOVA Assumptions

- Data is derived from a multivariate Gaussian distribution
- Each group has the same covariance matrix

There must be a better test out there

Slight Tangent - Independence Testing

- X and Y are independent if neither contains information about the other
- In other words,

$$F_{XY} = P(X \leq a \text{ and } Y \leq b) = P(X \leq a) \times P(Y \leq b) = F_X F_Y$$

$$F_{XY} = F_X F_Y$$

Note: These ideas and notation generalize for multivariate X and Y.

Distance Correlation (Dcorr)

$$\widehat{Dcov}_{xy} = \frac{1}{n^2}\operatorname{tr}(\mathbf{H}\mathbf{D}^{\mathbf{x}}\mathbf{H}\mathbf{D}^{\mathbf{y}}\mathbf{H})$$

$$\widehat{Dcorr}_{xy} = \frac{\widehat{Dcov}_{xy}}{\sqrt{\widehat{Dcov}_{xx} \times \widehat{Dcov}_{yy}}}$$

$$\mathbf{C}^{\mathbf{x}}_{ij} = \mathbb{I}_{i \neq j}\left(\mathbf{D}^{\mathbf{x}}_{ij} - \frac{1}{n-2}\sum_{t=1}^{n}\mathbf{D}^{\mathbf{x}}_{it} - \frac{1}{n-2}\sum_{t=1}^{n}\mathbf{D}^{\mathbf{x}}_{tj} + \frac{1}{(n-1)(n-2)}\sum_{t=1}^{n}\mathbf{D}^{\mathbf{x}}_{tt}\right)$$

$$Dcov_{xy} = \frac{1}{n(n-3)}\operatorname{tr}(\boldsymbol{C}^{\mathbf{x}}\boldsymbol{C}^{\mathbf{y}})$$

$$Dcorr_{xy} = \frac{Dcov_{xy}}{\sqrt{Dcov_{xx} \times Dcov_{yy}}}$$

Multiscale Graph Correlation (MGC)

- Compute local Dcorr **at all scales**
- Find scale with **max** smoothed test statistic
- Permutation test to determine p-value

Kernel Mean Embedding Random Forest (KMERF)

- Train random forest on X, compute kernel matrix
- Transform similarity kernel matrix to distance matrix
- Permutation test to determine p-value

Great, what now?

- Can reduce the k-sample testing problem to the independence problem

$$\mathbf{x} = \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_k \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} \mathbf{1}_{n_1 \times 1} & \mathbf{0}_{n_1 \times 1} & \cdots & \mathbf{0}_{n_1 \times 1} \\ \mathbf{0}_{n_2 \times 1} & \mathbf{1}_{n_2 \times 1} & \cdots & \mathbf{0}_{n_2 \times 1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_{n_k \times 1} & \mathbf{0}_{n_k \times 1} & \cdots & \mathbf{1}_{n_k \times 1} \end{bmatrix}$$

- Run any independence test

- ***Note: This process does not add any additional computational complexity to the independence testing algorithm***

Simulations

Definitions

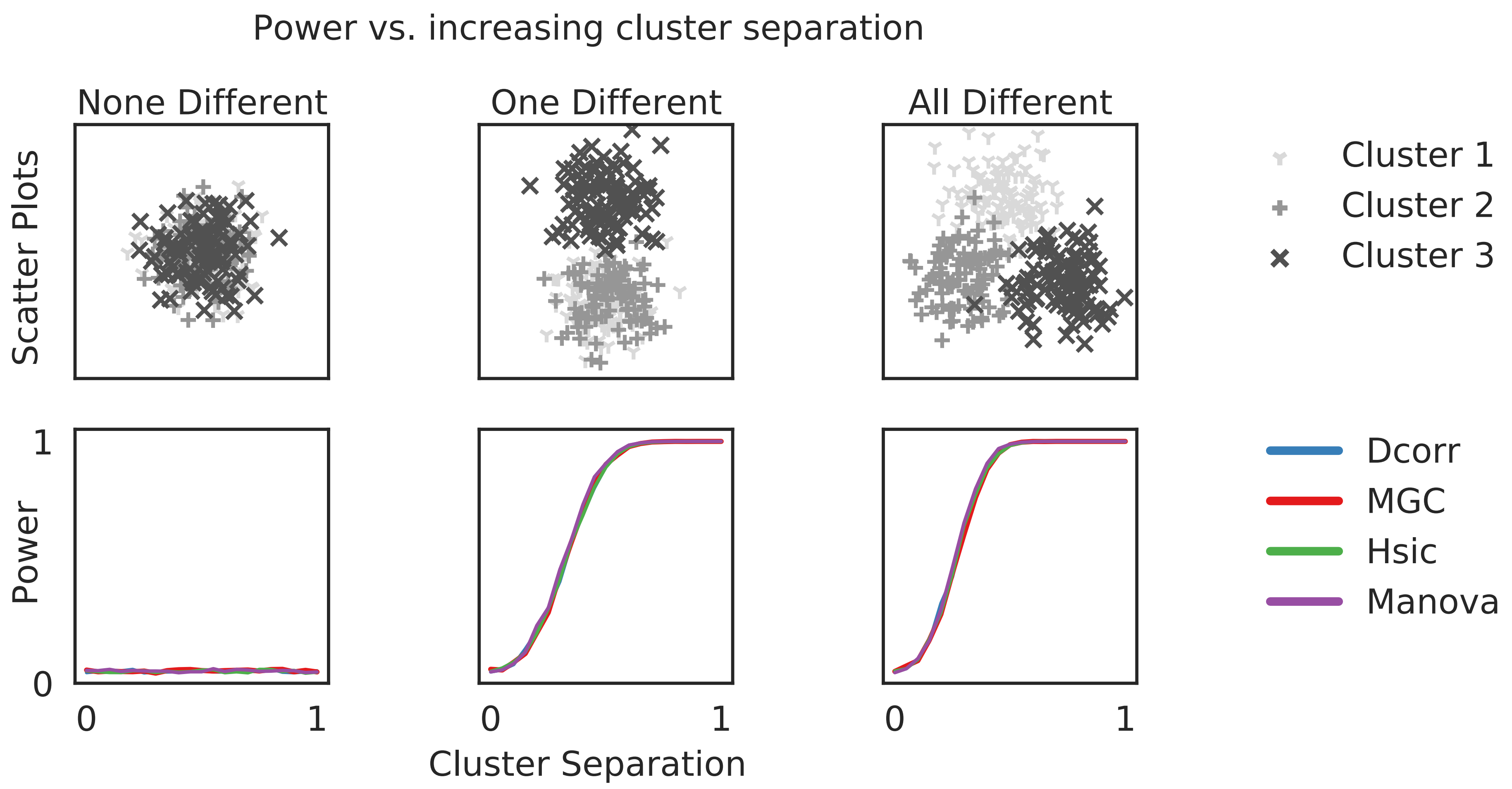
- **power** is the probability of rejecting the null when the alternative is true

$\beta_n(t)$: power of test statistic t given n samples

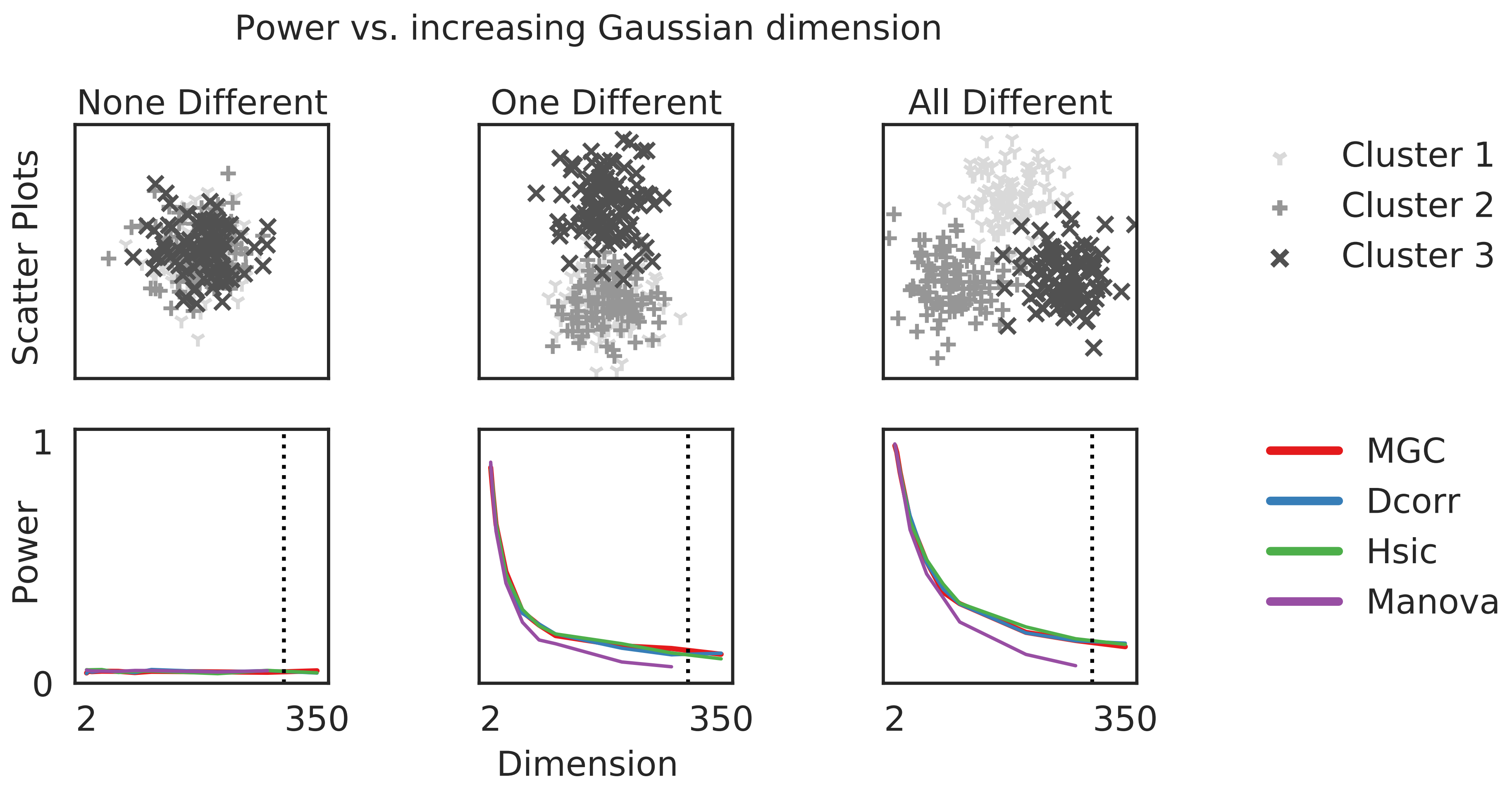
- **relative power** power of one approach minus power of another

$$\beta_n(t) - \beta_n(manova)$$

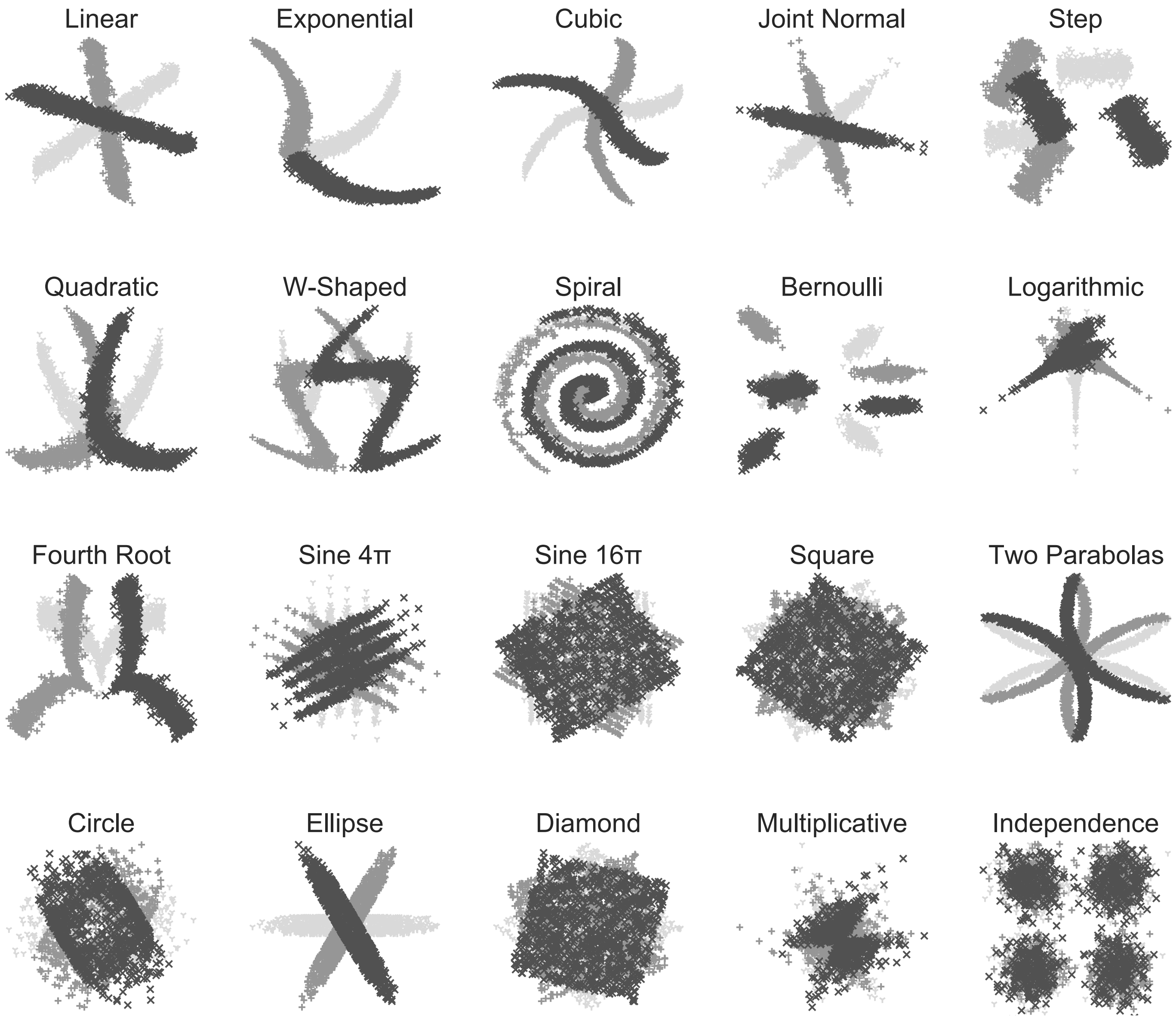
Optimal Settings for MANOVA (1D)

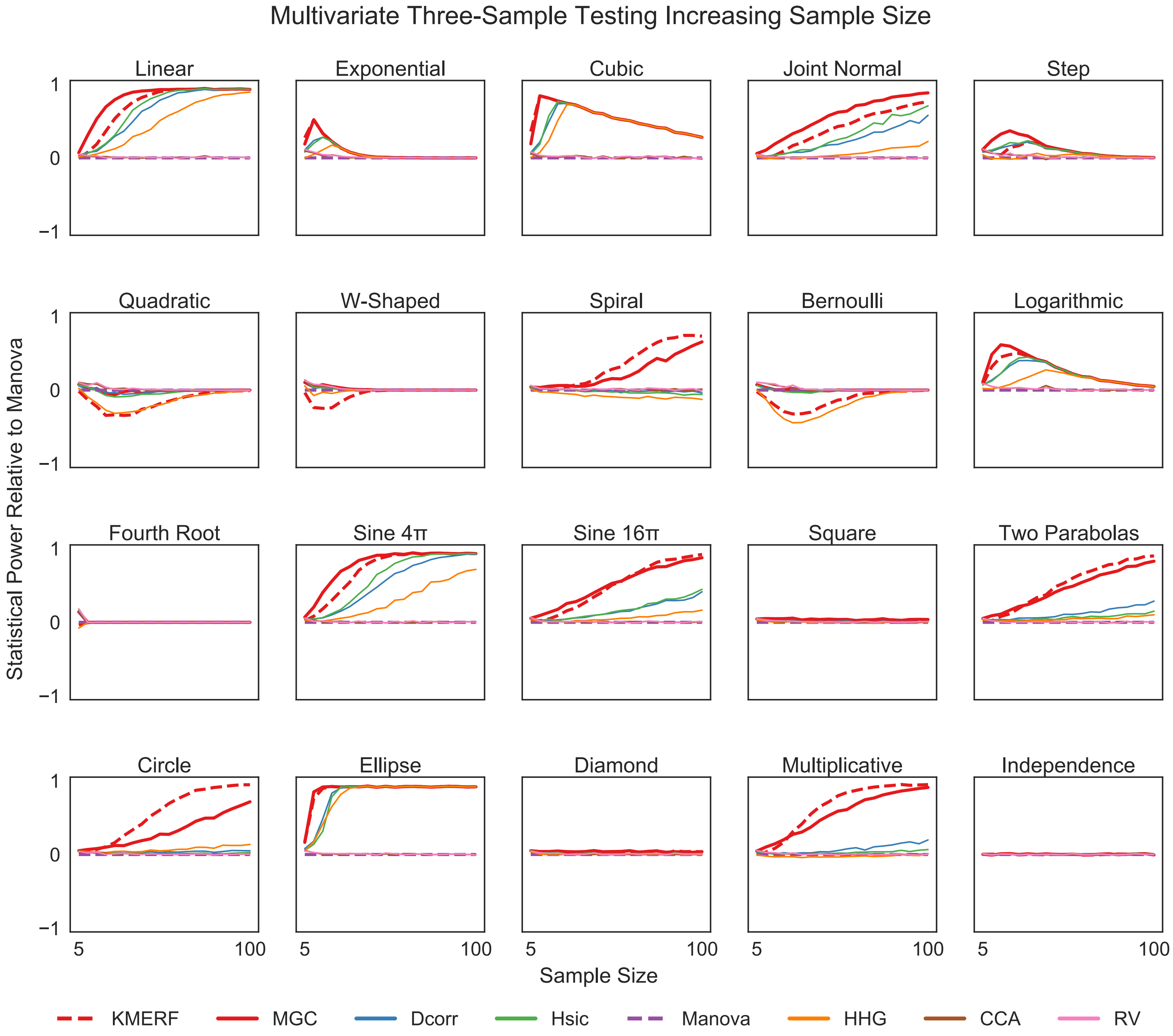


Optimal Settings for MANOVA (HD)



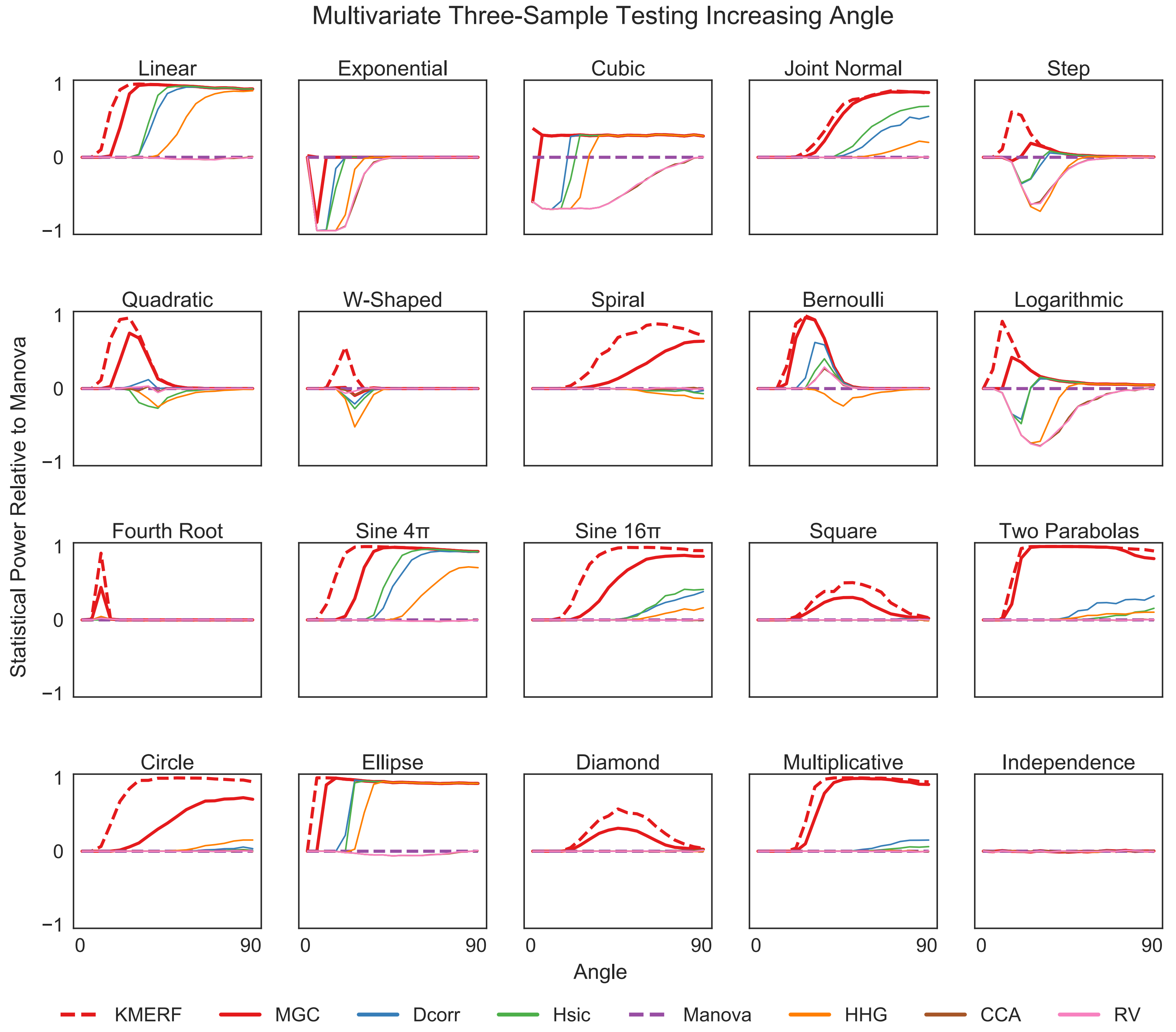
20 Different Functions (2D version)





Multivariate Three-Sample Testing Increasing Sample Size
Linear
Exponential
Cubic
Joint Normal
Step
Quadratic
W-Shaped
Spiral
Bernoulli
Logarithmic
Fourth Root
Sine 4π
Sine 16π
Square
Two Parabolas
Circle
Ellipse
Diamond
Multiplicative
Independence
Statistical Power Relative to Manova
Sample Size
1
0
−1
5
100
KMERF
MGC
Dcorr
Hsic
Manova
HHG
CCA
RV


Multivariate Three-Sample Testing Increasing Dimension
Linear
Exponential
Cubic
Joint Normal
Step
Quadratic
W-Shaped
Spiral
Bernoulli
Logarithmic
Fourth Root
Sine 4π
Sine 16π
Square
Two Parabolas
Circle
Ellipse
Diamond
Multiplicative
Independence
Statistical Power Relative to Manova
Dimension
1
0
−1
3
10
KMERF
MGC
Dcorr
Hsic
Manova
HHG
CCA
RV

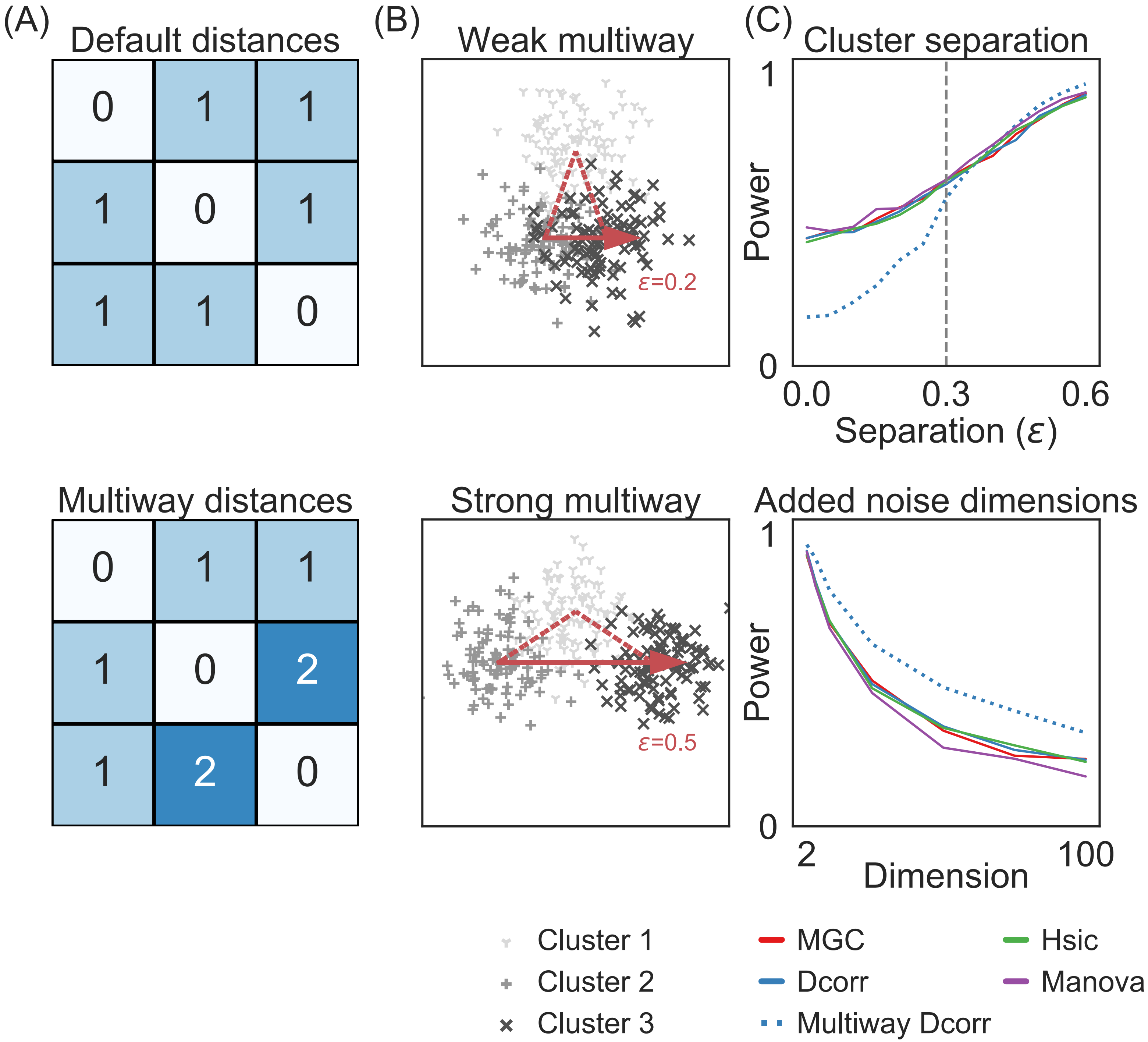


Multivariate Three-Sample Testing Increasing Angle
Linear
Exponential
Cubic
Joint Normal
Step
Quadratic
W-Shaped
Spiral
Bernoulli
Logarithmic
Fourth Root
Sine 4π
Sine 16π
Square
Two Parabolas
Circle
Ellipse
Diamond
Multiplicative
Independence
Statistical Power Relative to Manova
1
0
−1
0
90
Angle
KMERF
MGC
Dcorr
Hsic
Manova
HHG
CCA
RV

Multiway and Multilevel

Multiway Tests

- **Multiway**: More than one treatment group
- Instead of one-hot encoding, add 1’s columns of label matrix



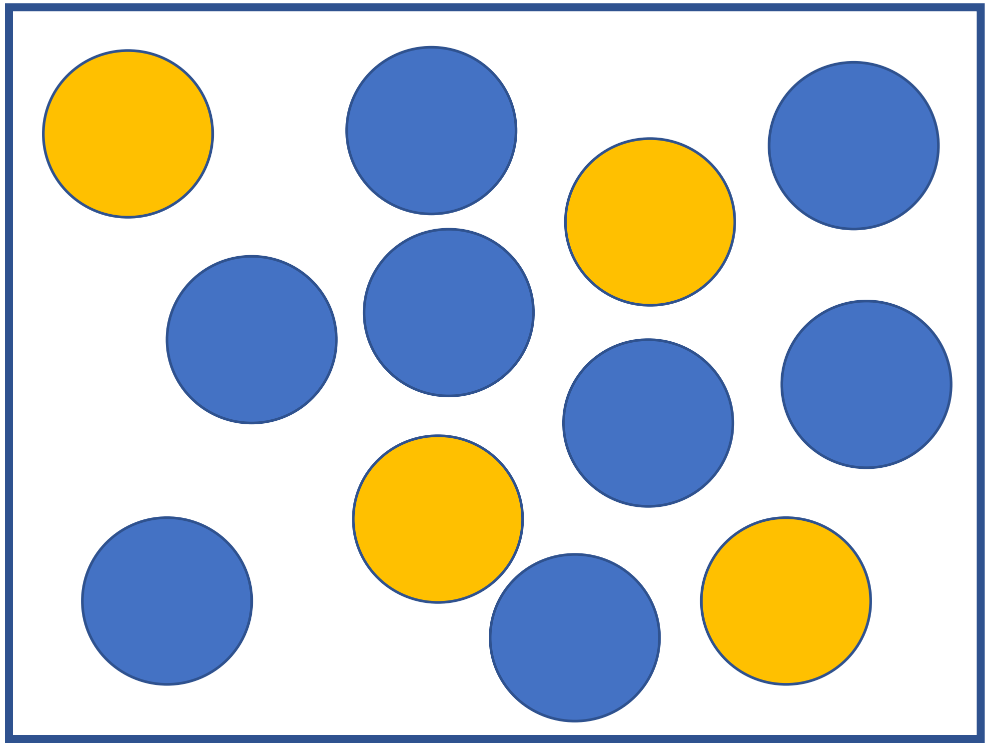
(A)
Default distances
0 1 1
1 0 1
1 1 0
Multiway distances
0 1 1
1 0 2
1 2 0
(B)
Weak multiway
ε=0.2
Strong multiway
ε=0.5
(C)
Cluster separation
Power
Separation (ε)
0.0 0.3 0.6
0 1
Added noise dimensions
Power
Dimension
2 100
0 1
Cluster 1
Cluster 2
Cluster 3
MGC
Dcorr
Multiway Dcorr
Hsic
Manova

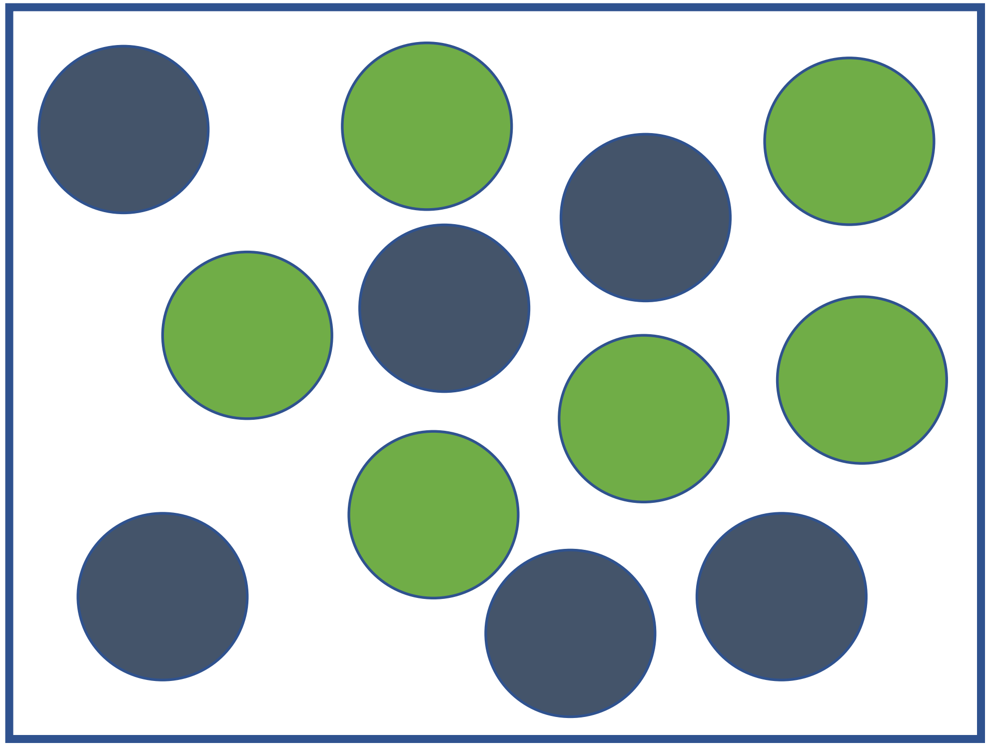
Multilevel Tests

- **Multilevel**: Samples are not always exchangeable with one another
- Need block permutation

Multilevel Tests

- **Multilevel**: Samples are not always exchangeable with one another





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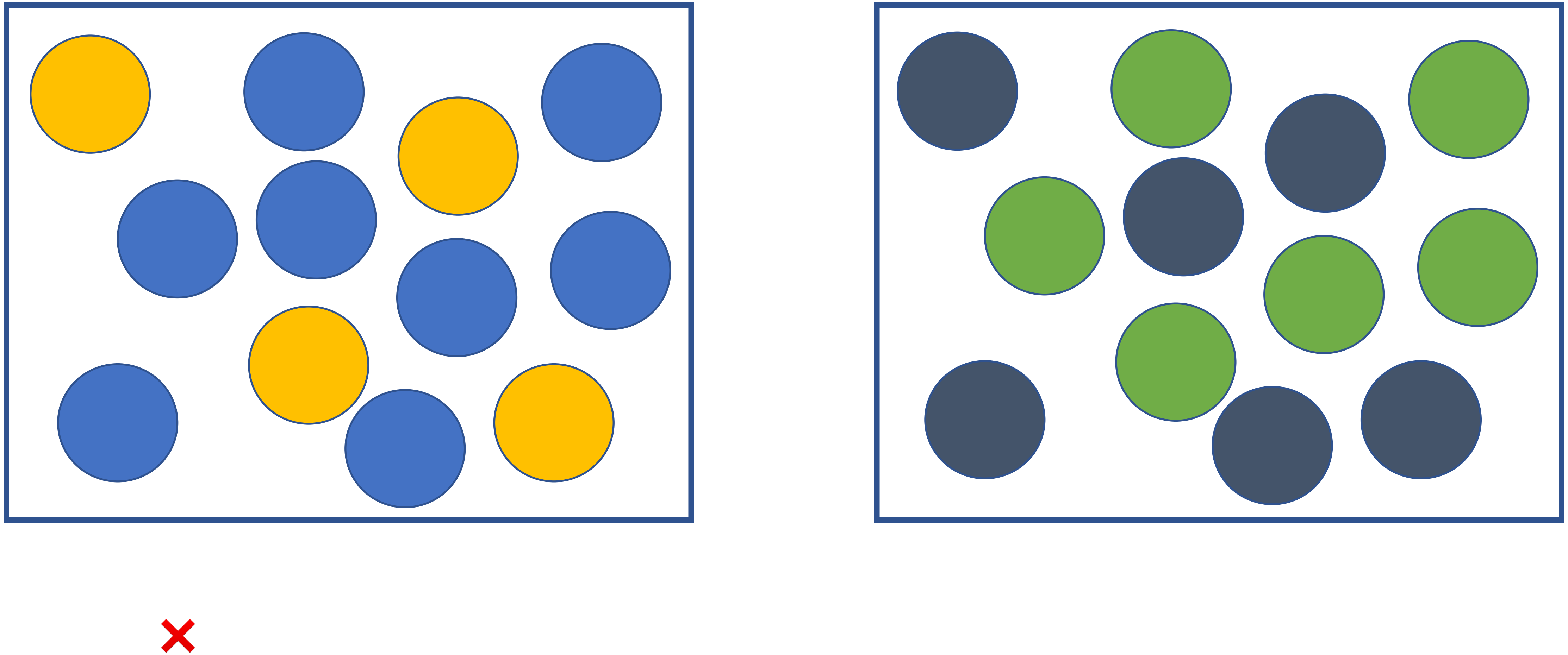
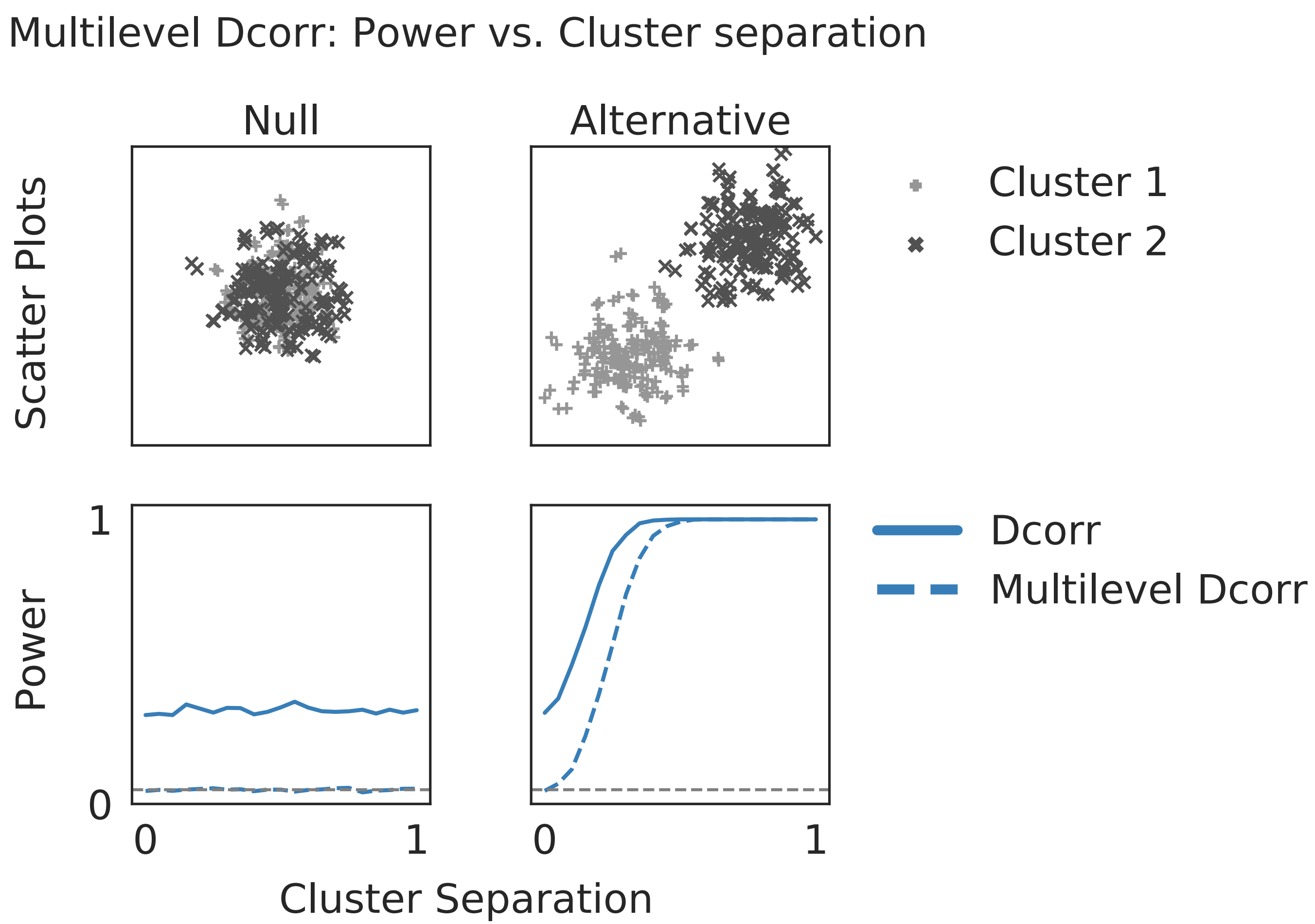
Multilevel Tests

- **Multilevel**: Samples are not always exchangeable with one another



Multilevel Tests

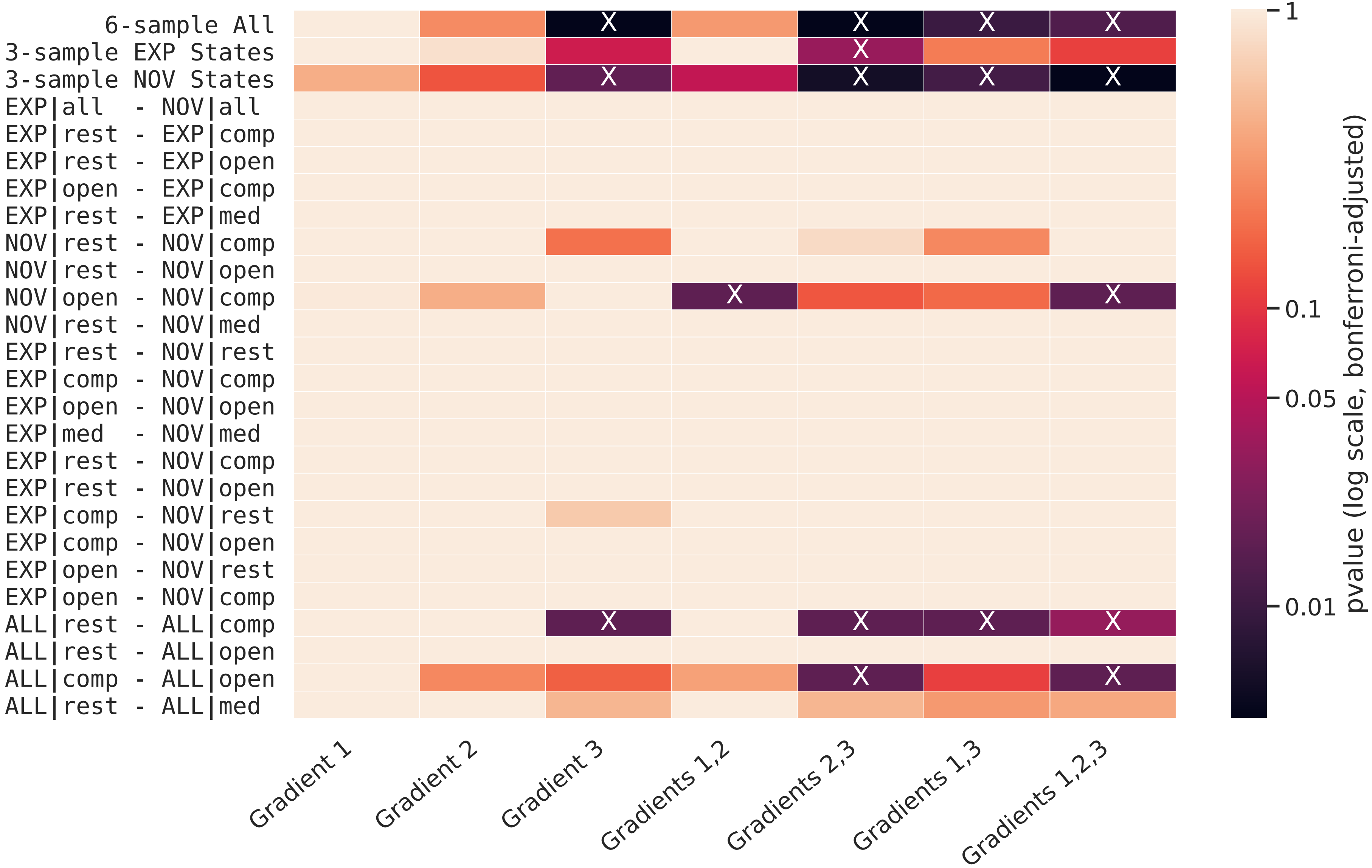


Real Data

The Procedure

- Data: 75 subjects – 28 experienced and 47 novice meditators
- 3 Recording sessions for each meditator
- Computed gradients and tested for difference between traits and novice
- This is a **multilevel and multiway test**

3^{rd} Embedding shows significance



Conclusions

- Presented several new k-sample tests using our framework
- At a simulation setting that fulfills MANOVA assumptions, our implementation performs as well or better
- Multiway tests give additional power when strong multiway effect is suspected
- Multilevel tests can now be performed

Next Steps

- All algorithms can be found in the hyppo package
    - Documentation
    - Install
    - Tutorials
- Paper

Email | Website | Twitter

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- …and the rest of the NeuroData Lab

DARPA

NIH National Institutes of Health

NSF

Microsoft Research

Questions?