Cluster analysis

Community health workers in a school, Rabai county, Kenya, September 2021

WASHA, Takwimu, UKZN, 25 August 2023

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PCA is easy to program and easy to implement and artful to interpret

2 TACTICS OF PCA

- Dimension reduction: How many principal components should we use?
- Discovery: What do the principal components mean?

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Principal component analysis uses two foundations of statistics, which come with assumptions

ASSUMPTIONS OF CANONICAL PCA

1. Linearity
2. Mean and variance sufficient statistics
3. Large variance mean important dynamics (high SNR)
4. Principal components are orthogonal

Quantitative analysis serve many important functions in health systems research

4 FUNCTIONS

1. Description
2. **Discovery – unsupervised machine learning**
    - Dimension reduction: low-dimensional representation of the observations that explain a large fraction of the total variance
    - **Cluster analysis:** homogeneous subgroups among the observations
3. Prediction
4. Causation

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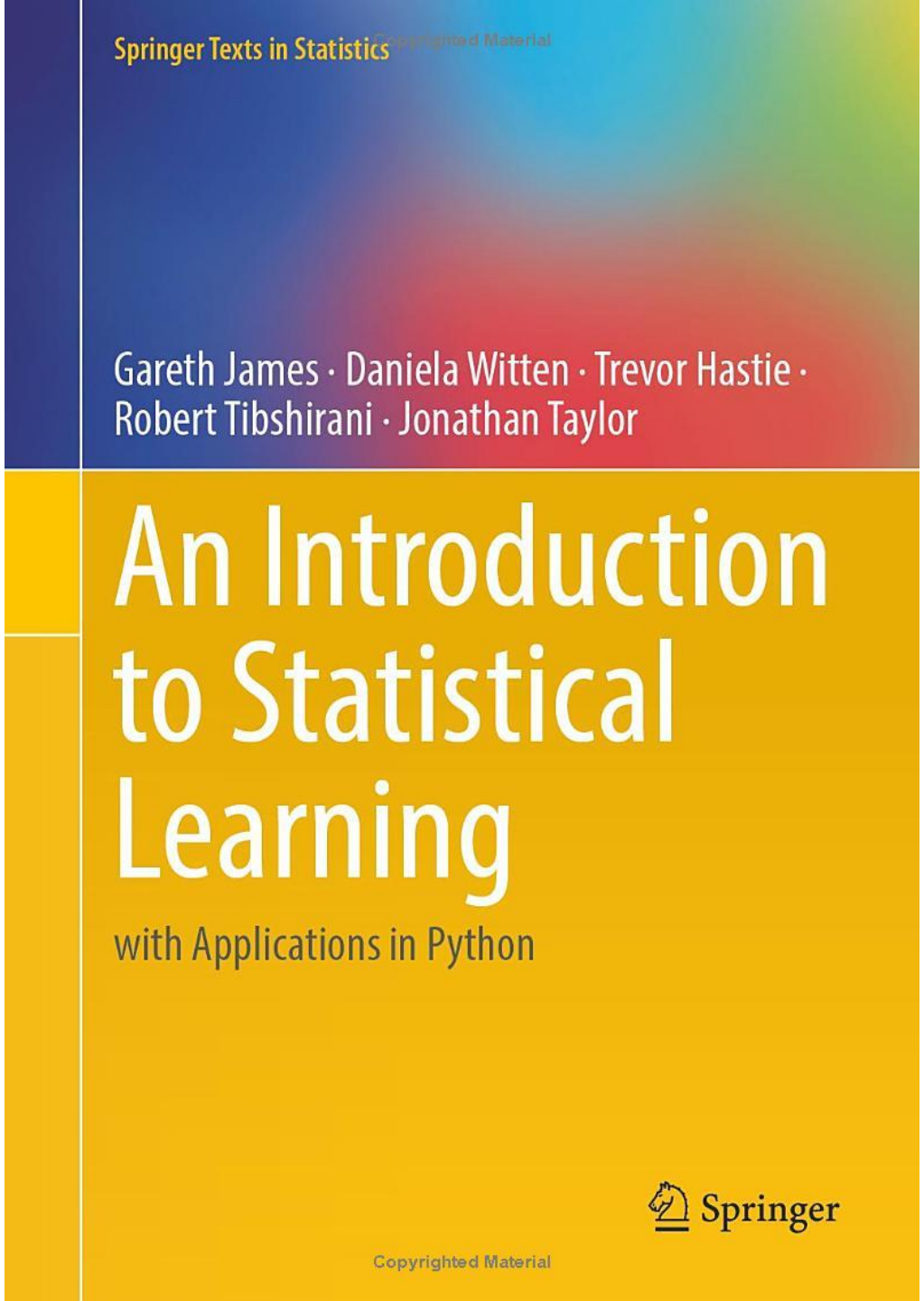
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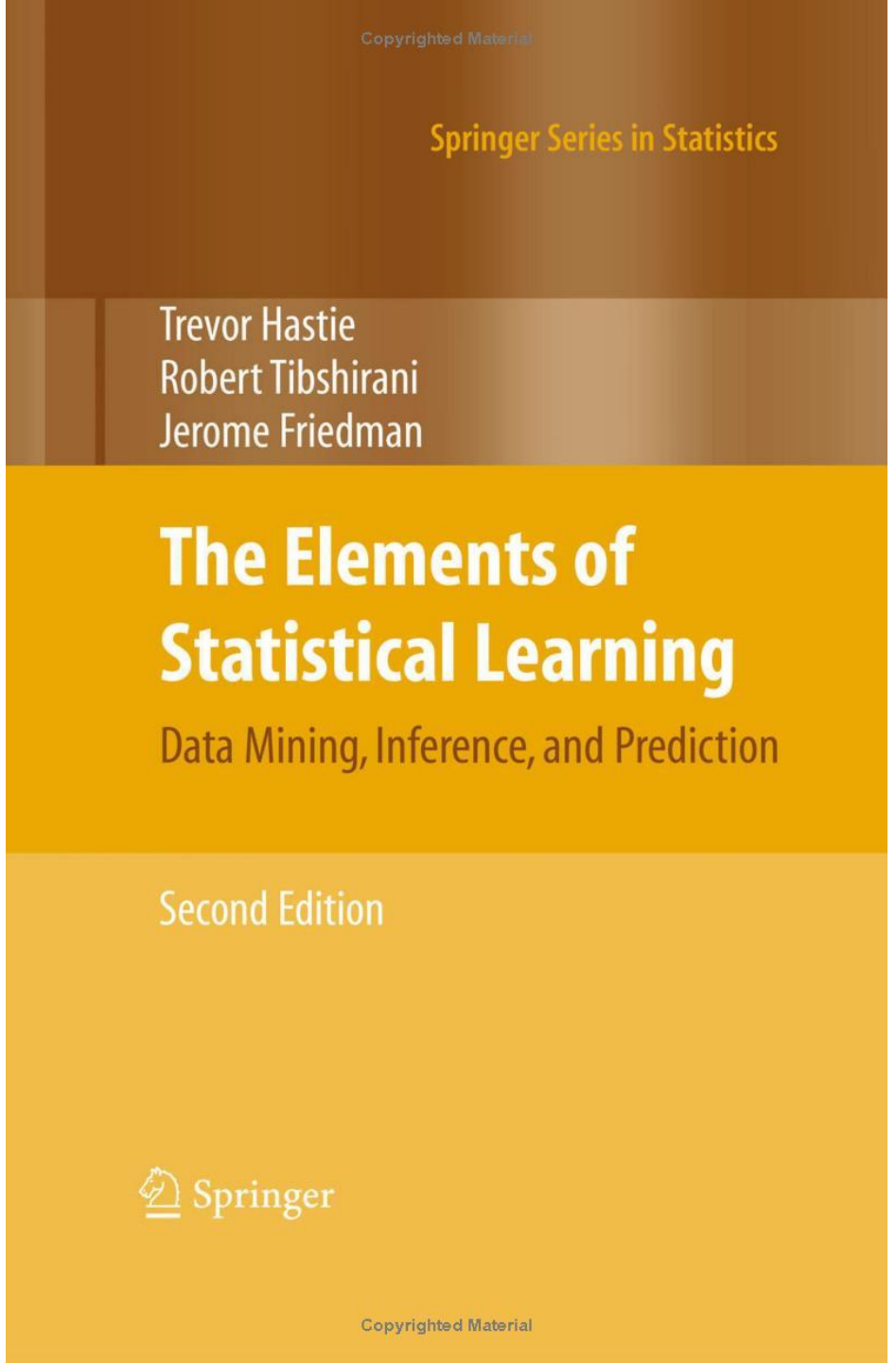
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K means rests on simple mathematical foundations

MATHEMATICAL INTUITION (I)

- Minimize the total within-cluster variation, summed over all *K* clusters

$$min_{C_1, C_2, \ldots C_K} \sum_{k=1}^{K} W(C_k)$$

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K means rests on simple mathematical foundations

MATHEMATICAL INTUITION (II)

- Minimize the sum of all the pairwise squared Euclidian distances between the observations in the k^{th} cluster, divided by the total number of observations in the k^{th} cluster – the summed over all K clusters

$$min_{C_1, C_2, \ldots C_K} \sum_{k=1}^{K} \frac{1}{C_k} W \sum_{i,i' \in C_k} \sum_{j=1}^{p} \left(x_{ij} - x_{i'j} \right)^2$$

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What PCA is for dimension reduction, k means is for cluster analysis

PROCEDURAL INTUITION

- Two properties:
  - Each observation belongs to at least one of the k clusters
  - No observation belongs to more than one cluster
- Steps:
  1. Choose *K*
  2. Randomly assign a number from 1 to K to each observation
  3. Iterate until the assignments stop changing:
     a. For each of the *K* clusters, compute the cluster centroid (vector of the *p* feature means)
     b. Assign each observation to the cluster whose centroid is closest (using Euclidian distance)

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How to choose the hyperparameter *K*?

INTUITION AND METRICS EXAMPLES (I)

- We have to quantify the goodness of a clustering
- All metrics capture some version of one or both of two high-level ‘goodness’ characteristics
  - Within: **cohesion** or **compactness** of clusters
  - Across: **separation** of clusters

$$\frac{(\alpha * separation)}{(\beta * compactness)}$$

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How to choose the hyperparameter *K*?

INTUITION AND METRICS EXAMPLES (II)

- **Silhouette coefficient** (SC) – uses the mean intracluster distance (a) and the mean nearest-cluster distance (b)

$$\frac{(b-a)}{\max(a,b)}$$

- **Dunn index (DI)**

$$\frac{(\min separation = \min pairwise\ intercluster\ distance)}{(\max diameter = \max intracluster\ distance = \ compactness)}$$

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What clusters of chronic disease dominate in India?

METHODS – FINGER EXERCISE (I)

1. Data source: National Family Health Survey – 639,661 women
2. Variables: biomarkers and anthropometric measures that indicate major chronic conditions – continuous variables
   - Height and weight
   - Waist and hip circumference
   - Hemoglobin
   - Random blood glucose
   - Systolic and diastolic blood pressure

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What clusters of chronic disease dominate in India?

METHODS – FINGER EXERCISE (II)

3. Data preprocessing:
   - Observations removed because of implausible values (14 weight or height, 5 blood sugar, 11 systolic or diastolic blood pressure)
   - PCA: first five principal components using Kaiser's criterion – from 8 to 5 dimensions
4. Cluster analysis:
   - K means
   - *NbClust* R package for k hyperparameter optimization, using 26 cluster performance indices – majority vote

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5 clusters of chronic conditions emerge among women in India

METHODS – FINGER EXERCISE (III)

Index name	# clusters
KL	5
CH	5
Hartigan	4
CCC	5
Scott	5
Marriot	5
TrCovW	5
TraceW	5
Friedman	5
Rubin	5
Cindex	4
DB	5
Silhouette	2
Duda	2
PseudoT2	2
Beale	2
Ratkowsky	5
Ball	3
PtBiserial	5
Frey	1
McClain	2
Dunn	9
Hubert	0
Sdindex	5
Dindex	0
SDbw	10

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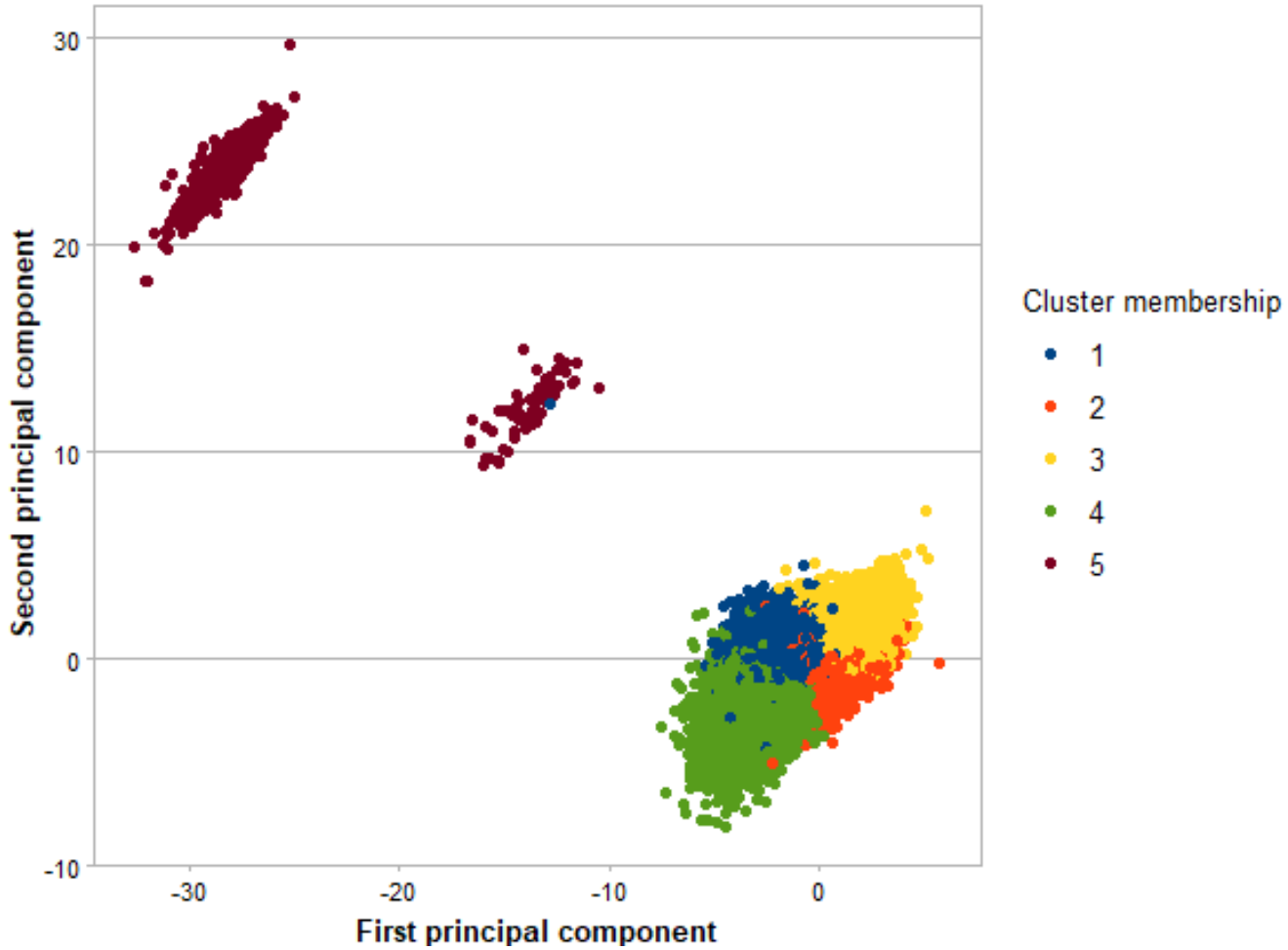

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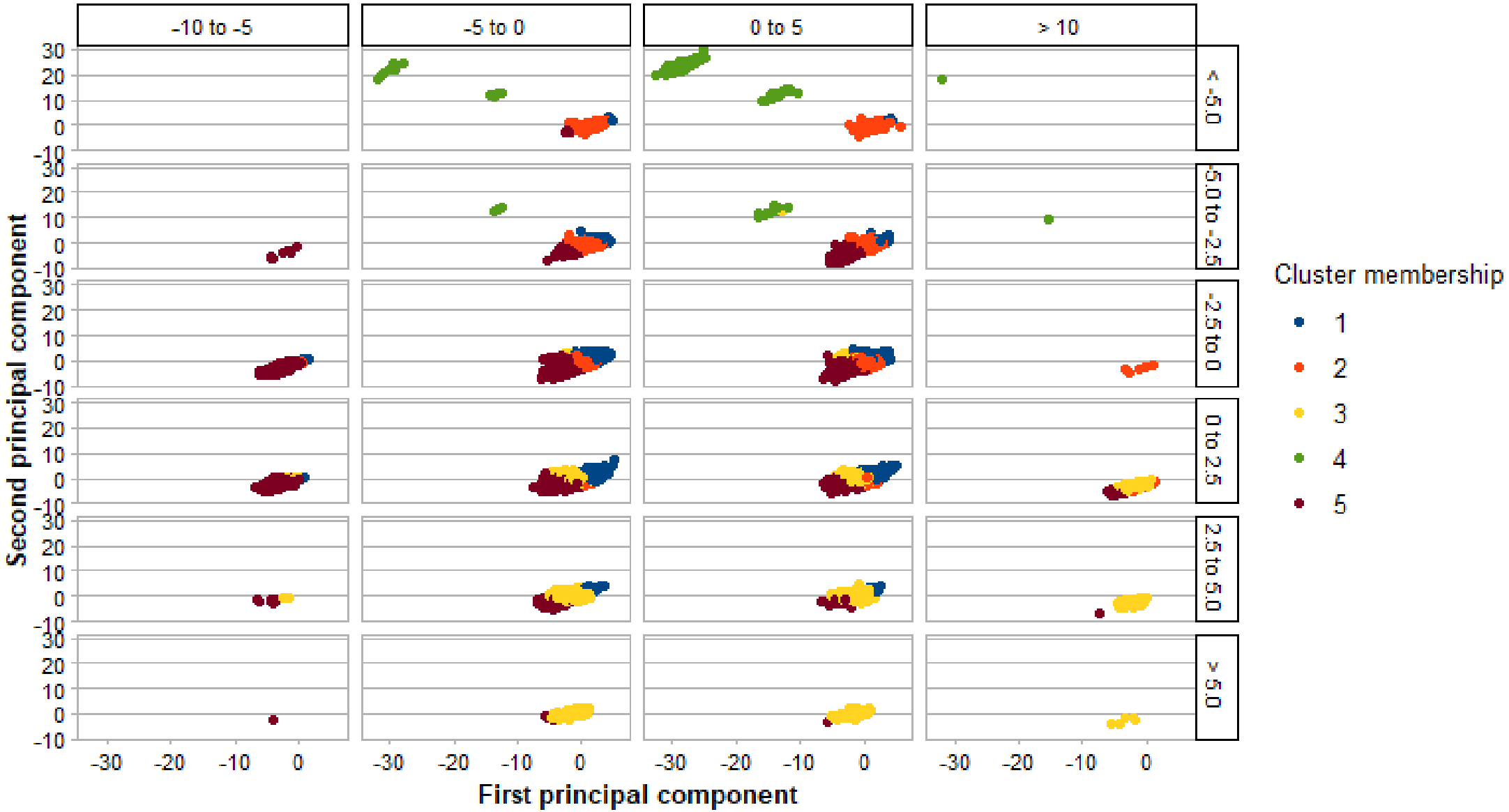
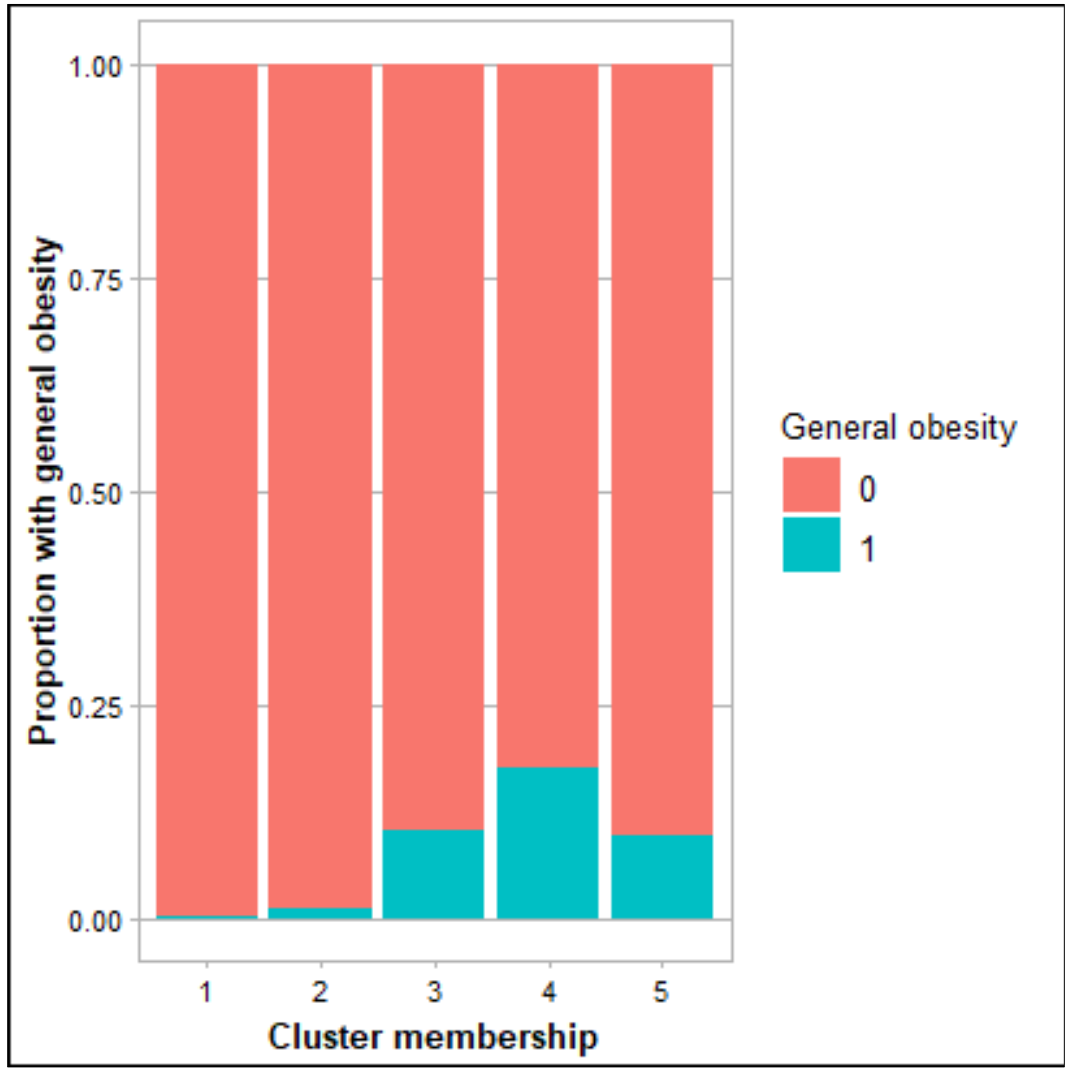

-10 to -5
-5 to 0
0 to 5
> 10
< -5.0
-5.0 to -2.5
-2.5 to 0
0 to 2.5
2.5 to 5.0
> 5.0
Second principal component
First principal component
Cluster membership
1
2
3
4
5



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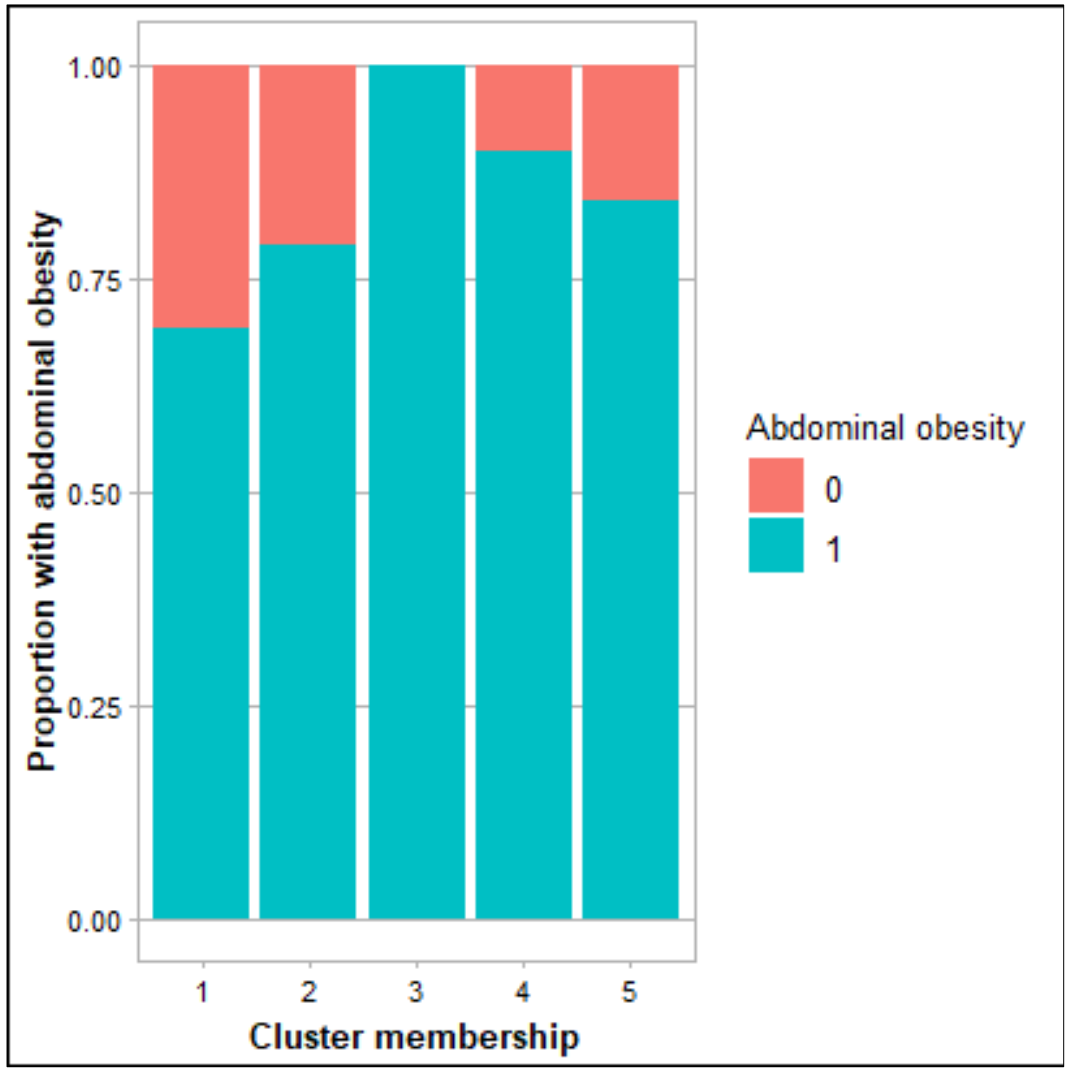

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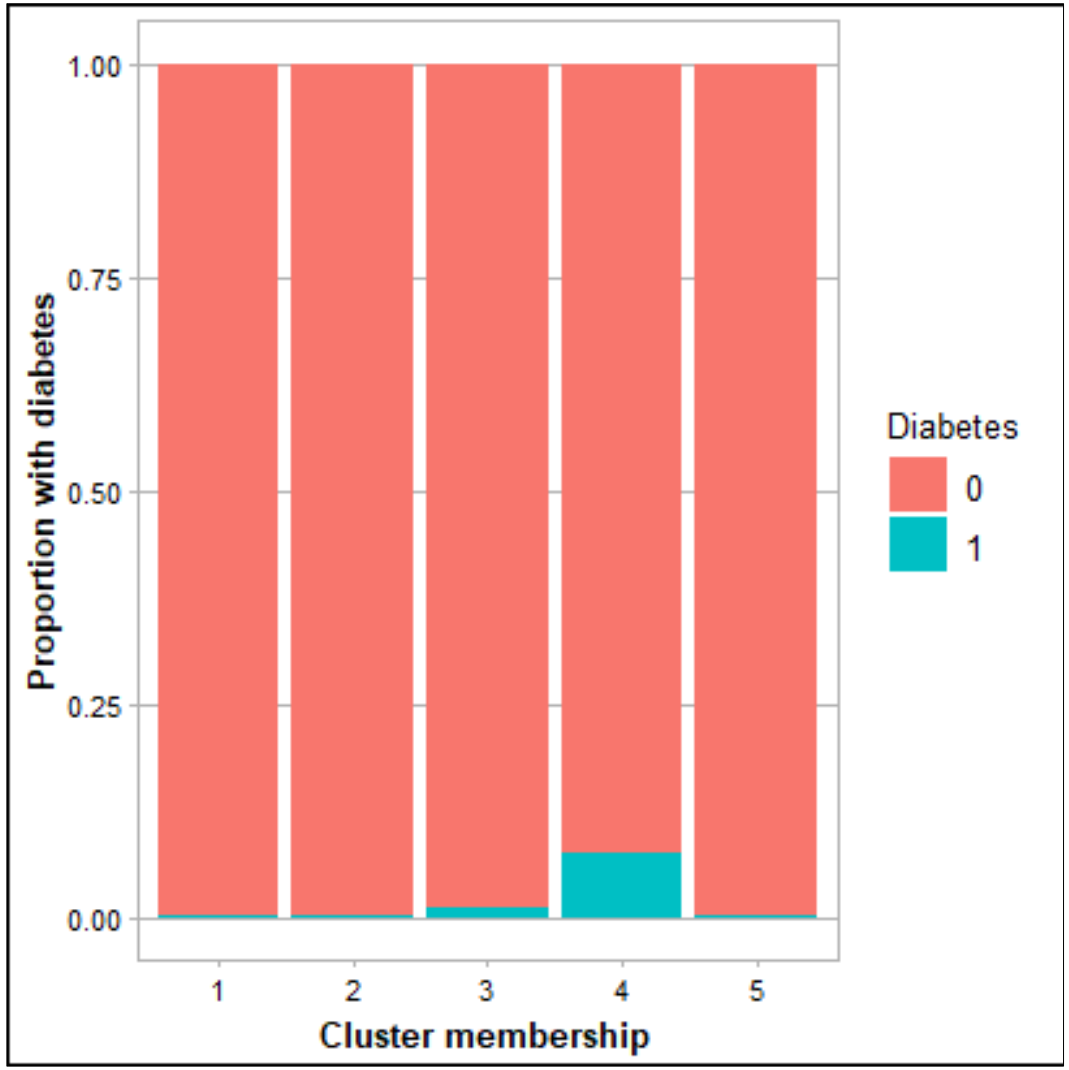

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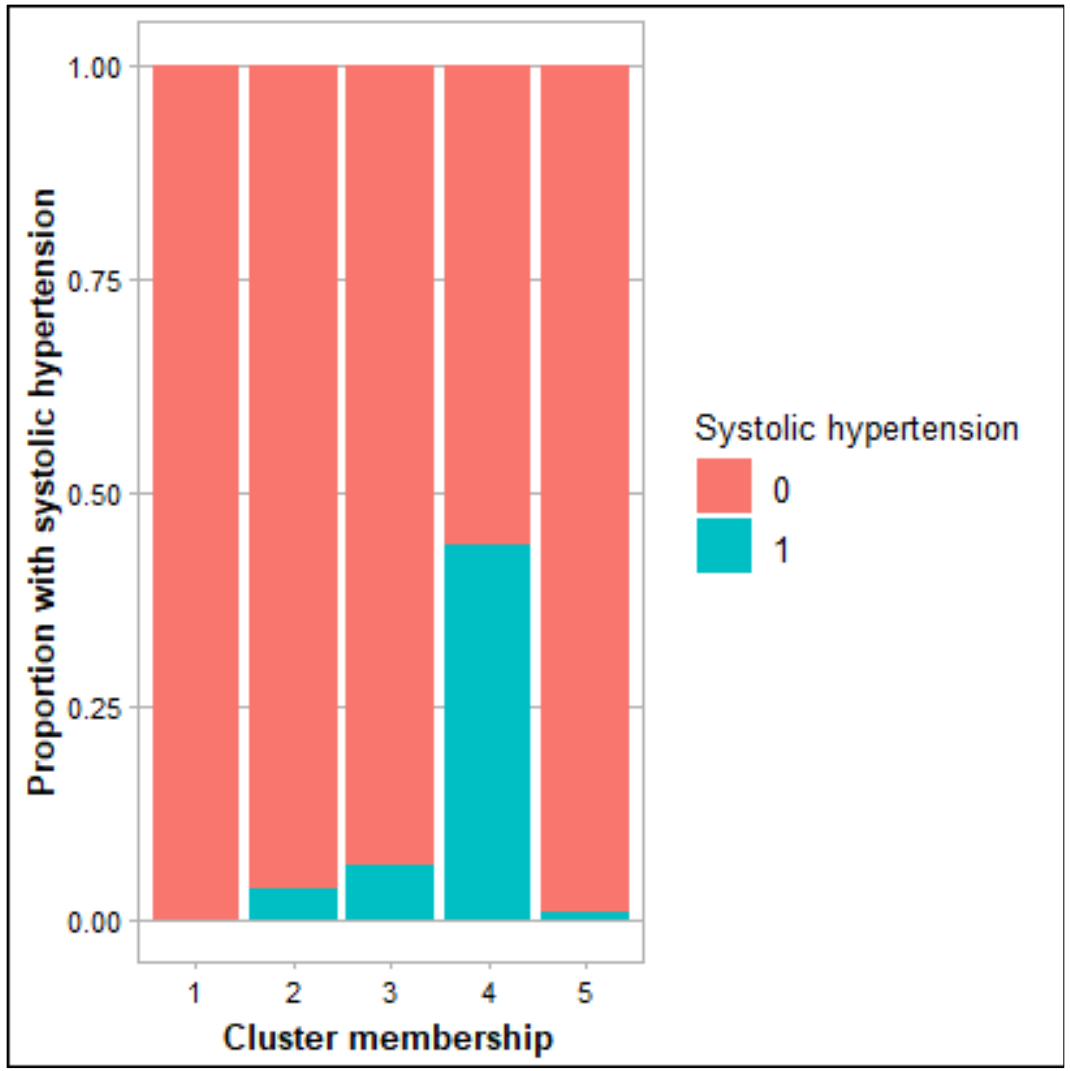

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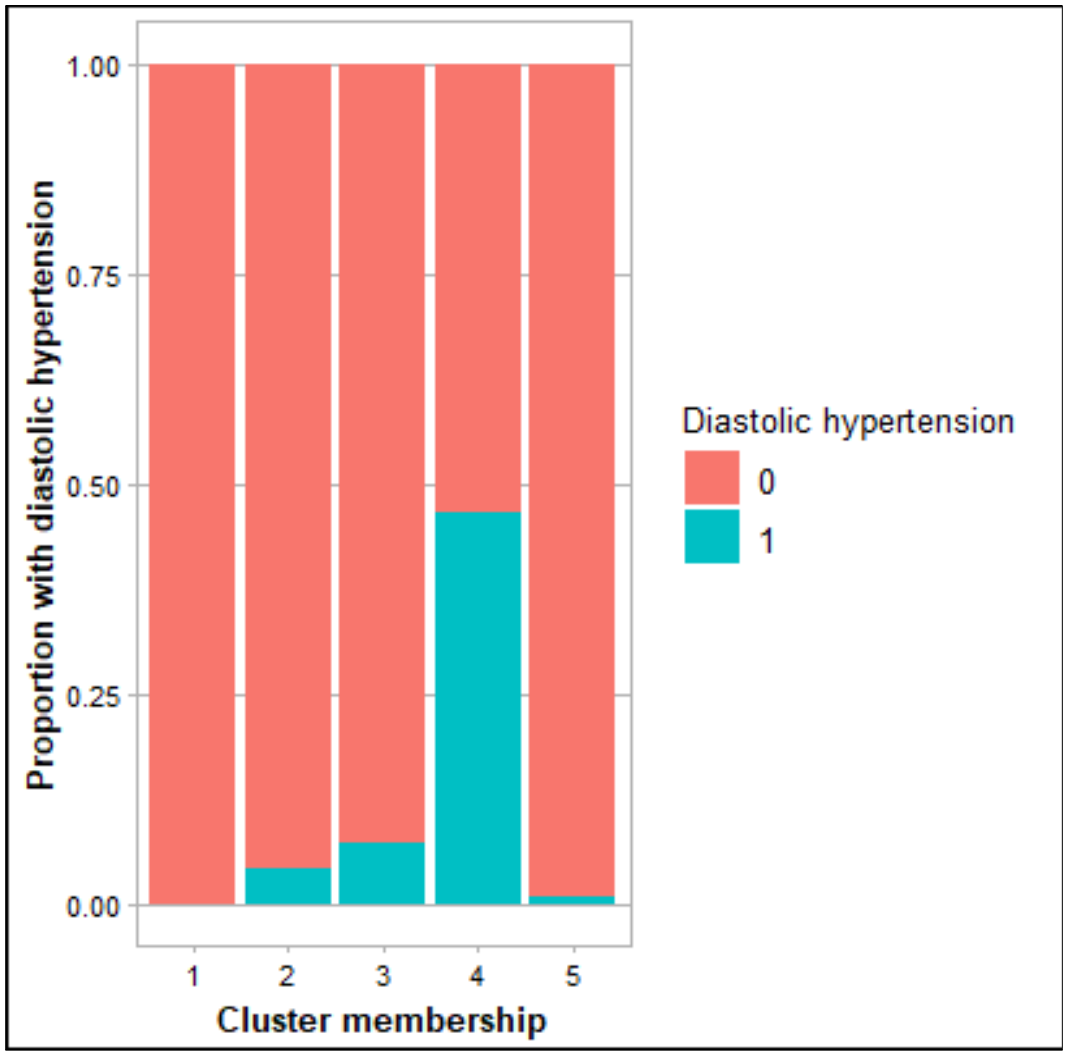

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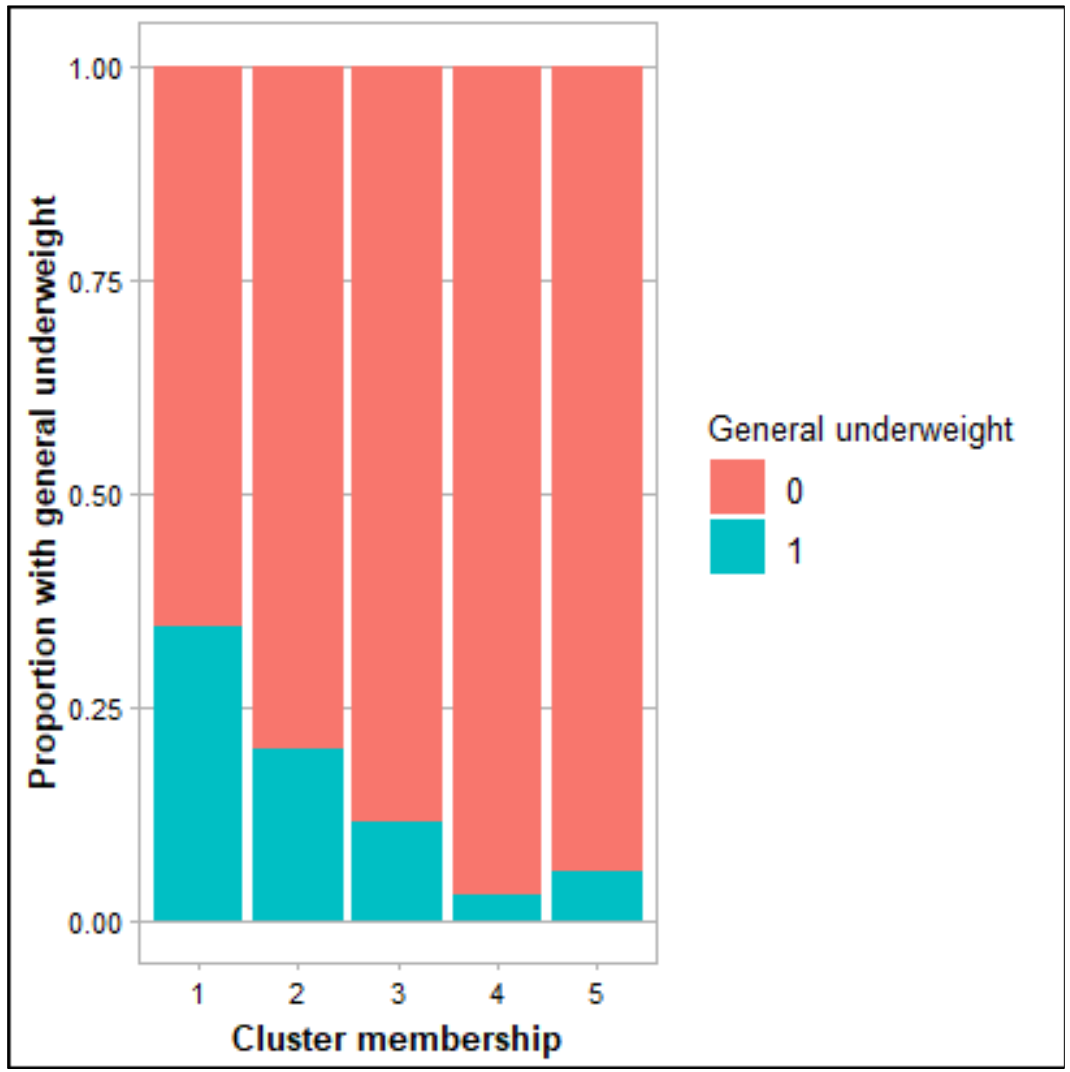

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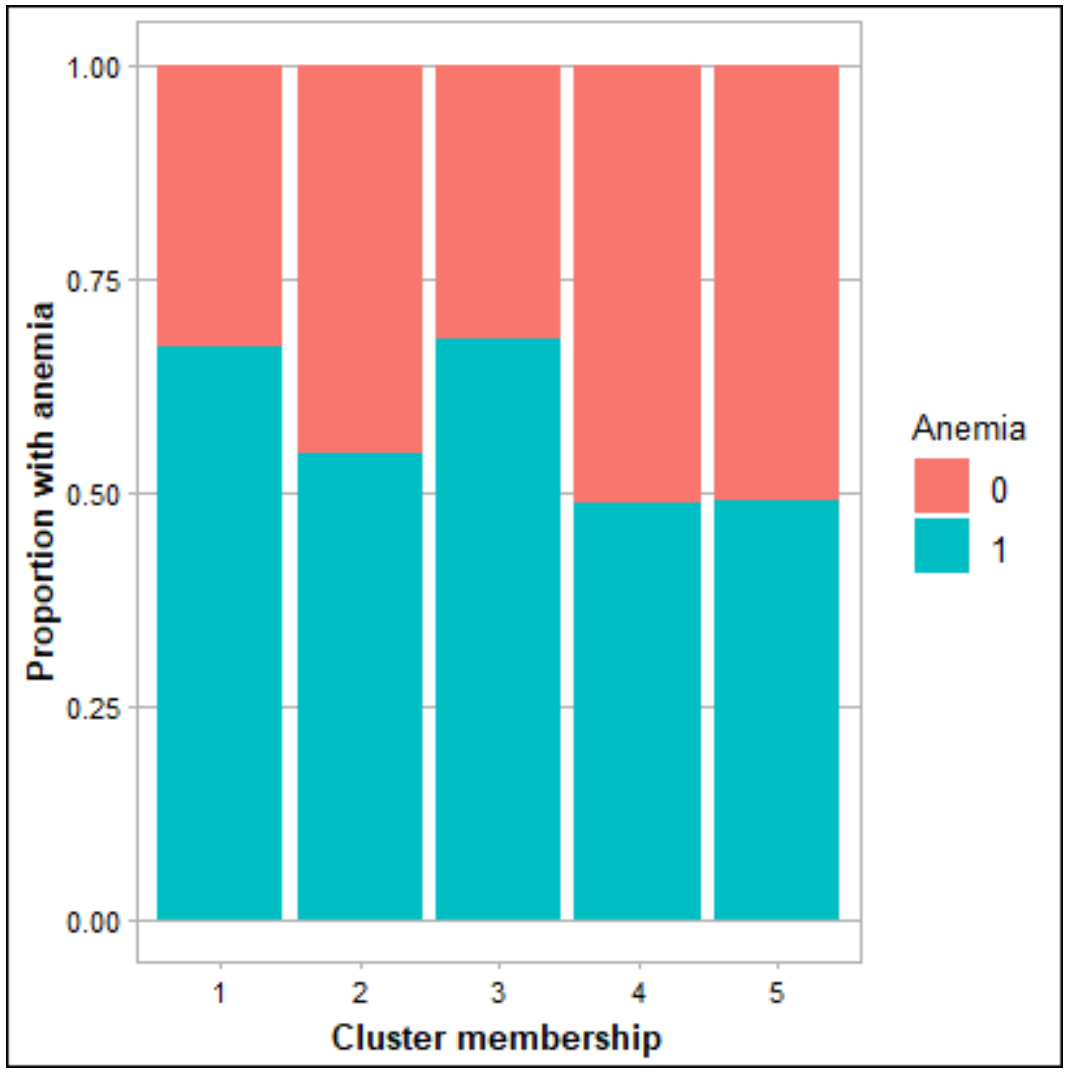

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What factors determine cluster membership?

METHODS – FINGER EXERCISE (IV)

5. Regression:
   - Multinomial logistic regression, using the *nnet* R package
   - Dependent variable: cluster membership
   - Independent variables: socio-demographic
     - Age
     - Education
     - Rural vs urban
     - Wealth
     - Religion (Hindu, Buddhist, Muslim, Sikh, Christian, Jain, Jewish, Zoroastrian, other, none)
   - Causal intention

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	Cluster membership (reference: cluster 1)			
	Cluster 2	*Cluster 3*	*Cluster 4*	*Cluster 5*
Age (years)	1.055***	1.038***	1.165***	1.084***
	(0.0004)	(0.005)	(0.001)	(0.0004)
Education (years)	0.986***	1.063***	1.007***	1.031***
	(0.001)	(0.010)	(0.001)	(0.001)
Wealth index (standard deviation)	0.910***	1.412***	1.443***	1.628***
	(0.004)	(0.051)	(0.006)	(0.005)
Rural *Residence (reference: urban)*	1.000***	0.951***	0.990***	1.116***
	(0.009)	(0.091)	(0.012)	(0.009)
Religion *(reference: Hindu)*				
Muslim	1.124***	1.373***	1.558***	1.522***
	(0.011)	(0.116)	(0.015)	(0.011)
Christian	1.289***	0.986***	1.570***	1.290***
	(0.013)	(0.165)	(0.018)	(0.014)
Sikh	0.919***	1.170***	2.189***	1.768***
	(0.030)	(0.252)	(0.030)	(0.025)
Buddhist	1.260***	0.915**	1.810***	1.228***
	(0.033)	(0.410)	(0.040)	(0.035)
Jain	1.290***	0.018***	1.199***	1.013***
	(0.112)	(0.00005)	(0.128)	(0.105)
Jewish	0.003***	0.526***	0.029***	1.334***
	(0.00000)	(0.00001)	(0.00000)	(0.00001)
Zoroastrian	4.175***	0.580***	3.354***	3.313***
	(0.257)	(0.0002)	(0.278)	(0.282)
No religion	2.492***	0.112***	5.235***	2.173***
	(0.168)	(0.0002)	(0.193)	(0.186)
Other religions	1.860***	0.190***	2.425***	1.505***
	(0.031)	(0.001)	(0.041)	(0.036)
Constant	0.244***	0.001	0.003	0.056***
	(0.018)	(0.196)	(0.027)	(0.019)

Different families of cluster analysis are useful for particular applications

TYPES

- **Centroid-based** (k means, medians, medoids …)
- **Distribution-based** (Gaussian, Bernoulli … mixture models)
- **Density-based** (HDBSCAN, DBSCAN, …)
- **Hierarchical** (trees)
- …

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How do health behavioral risks cluster?

BERNOULLI MIXTURE MODEL IN NAMIBIA