A Machine Learning Approach for Detecting Groundwater Runoff Connectivity

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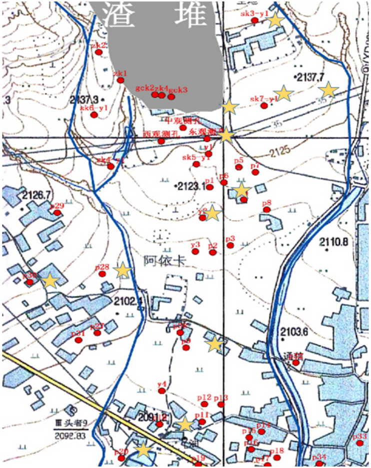
Research Background

Water samples were collected from 12 underground wells in Zhehai mining area, Yunan Province, China, and three samples were collected from each well in different time. Bacteria DNA in the water samples were sequenced.



sampling point	sample numbers
sk3	a
sk7	b
sk12	c
east observation point	d
leachate	e
y2	f
p6	g
p9	h
p10	i
p20	j
p28	k
p30	l

Research Purposes

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- Investigate the performance improvement of the cluster analysis.

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- **Refine** the clustering results referring to environmental parameters.

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- Partition clustering using K-mean and K-medoids (K-medoids is also called PAM - partitioning around medoids)

Hierachical Clustering Results

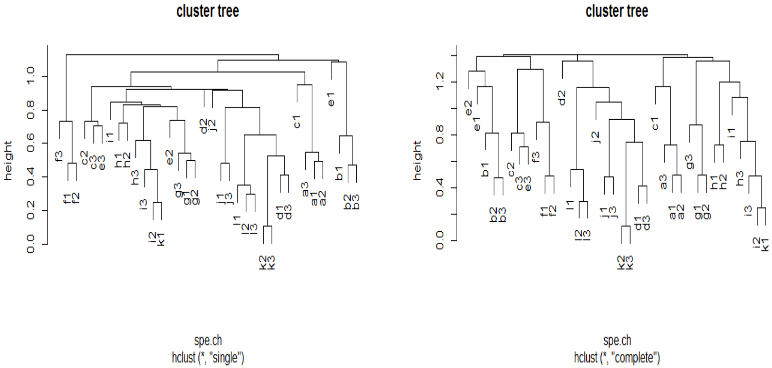

Figure 2: The cluster trees of min cluster (left) and max cluster (right)

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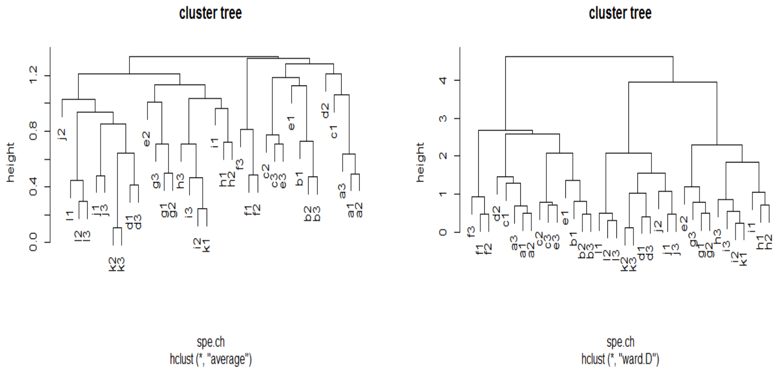

Figure 3: The cluster trees of mean cluster (left) and ward minimal variance cluster (right)

Evaluation of the Results

Calculate Pearson correlation coefficient, represented in Shepard. The larger, the better.

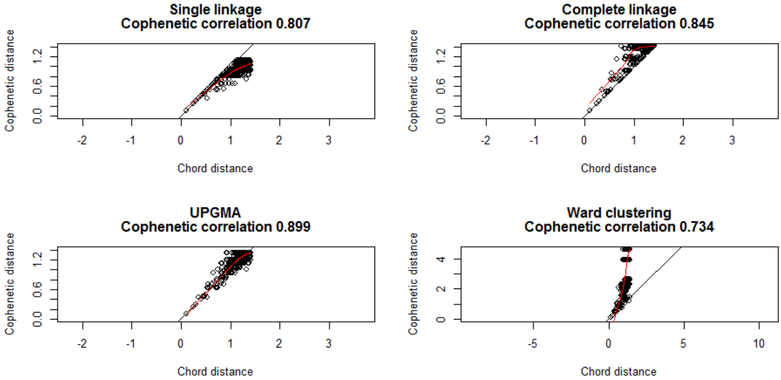

Figure 4: Shepard diagrams for each hierarchical analysis

Clustering Results

Calculate level of integration values to cut the tree, each subtree is a cluster.

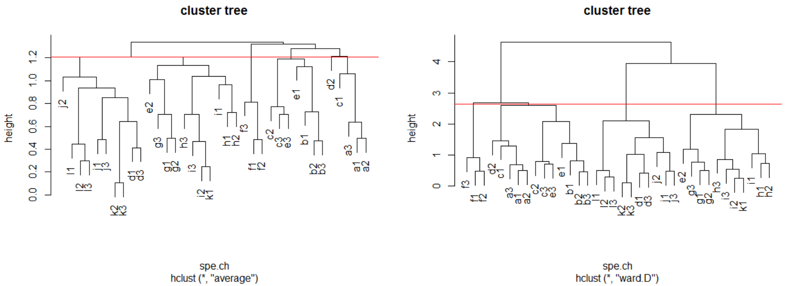

Figure 5: Clustering result, average clustering (left), and ward clustering (right)

Clustering Results

Each row represent one hierarchical analysis (min, max, average, and ward), and each column represents a cluster.

f	b	a	c	k、l、d、j	g、h、i
f、c	b、e	k、l、d、j	g、h、i、a	N/A	N/A
f	a、b、c、e	k、l、d、j	g、h、i	N/A	N/A
f	a、b、c、e	k、l、d、j	g、h、i	N/A	N/A

Figure 6: Clustering result

Partition Clustering Results

K-mean and PAM (or K-medodis). Iteratively experiment different k from 2 to 10 and evaluate the optimal K with SSI values.
PAM: {{a}, {b}, {k, l, j}, {g, h, i, f}}
K-mean (K = 4): {{a}, {b, c, d, e, f}, {k, l, j}, {g, h, i}}
K-mean (K = 6): {{a}, {b, c, e}, {h,i}, {g}, {f}, {k, l, j, d}}

Refine Results with Environmental Parameters

Understand how the environment such as heavy metal ion impact to the clustering. If two wells are connected, their heavy metal ion should impact the both of them.

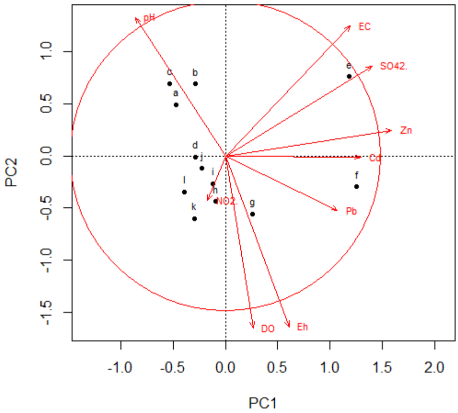

Figure 7: PCA on environmental parameters to clustering

Ordination with NMDS

Final clustering result: {{a, b, c, d, e}, {f}, {k, l, j}, {g, h, i}}

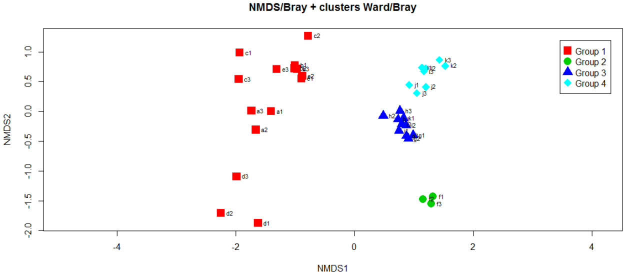

Figure 8: NMDS + Ward cluster.

Validation

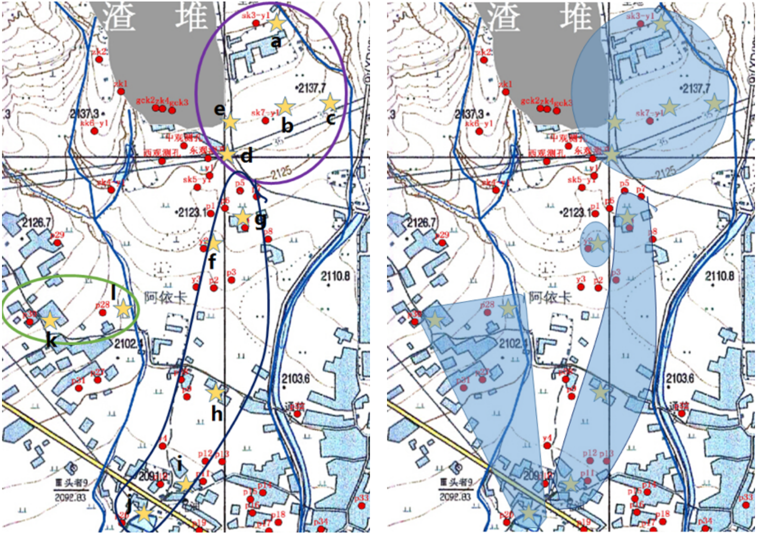

Figure 9: The distribution of groundwater derived from (a) physical and chemical experiments, and (b) ordination + clustering method.

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- More samples, more scenarios should be investigated.