

Clustering Considerations for Machine Learning

With examples from exploration data

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Key messages

- Focus is only on clustering
- Understand internals to maximise ML effectiveness
- Classification is a big field
- Data analysis is not for the faint-hearted
- Usage with some example exploration data

Machine Learning

Classification:

Creating meaningful groups out of a collection of objects

Build the Model:

Feature extraction to enable effective identification of new objects

Identification:

Use the model to identify new objects to one of the groups

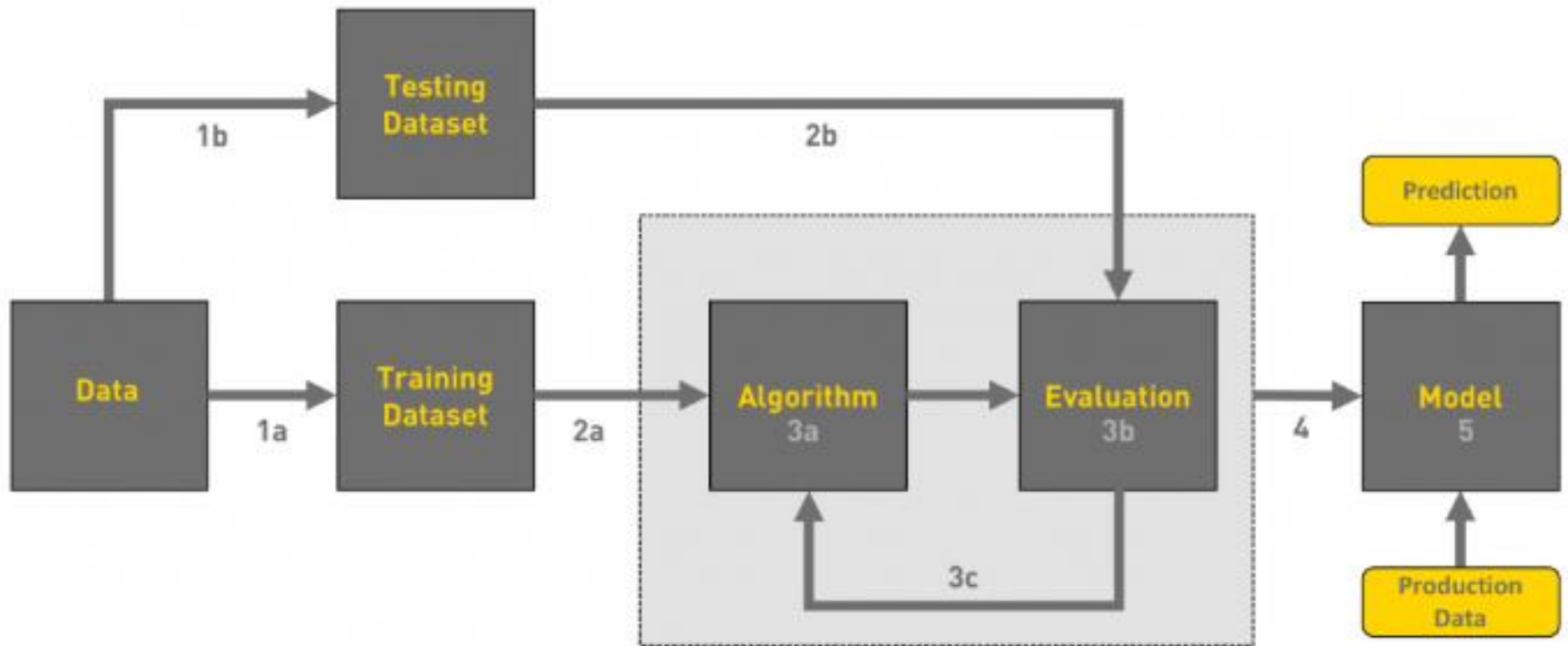
Unsupervised learning

Training
(Model building)

Testing

Supervised learning

The Machine Learning Workflow



<https://towardsdatascience.com>

Multivariate methods for classification and dimensionality reduction

- Cluster analysis
 - *Finding “natural” or pre-determined groups in datasets*
- Principal components analysis
 - *Reducing the dimensionality of a data set by finding a smaller set of variables that still represents it*
- Factor analysis
 - *For data sets where a large number of observed variables are thought to reflect a smaller number of unobserved/latent variables.*
- Multi dimensional scaling
 - *Technique for visualising the level of similarity of samples transformed onto a 2D plane*
- Linear & Multiple Regression
 - *One or more independent variables are used to predict the value of a dependent variable*

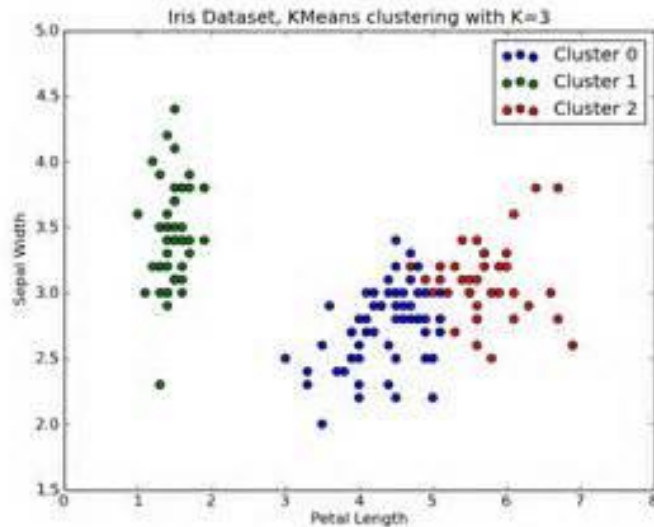
Some approaches to Clustering

- K-Means
 - *Iterative computing of distances between points and group means. Requires specification of number of groups.*
- Mean Shift Clustering
 - *Sliding iterative method to find point groups of higher mean density.*
- Density-Based Spatial Clustering of Applications with Noise (DBSCAN)
 - *Similar to Mean Shift but will identify noise and outliers.*
- Expectation–Maximization (EM) Clustering using Gaussian Mixture Models (GMM)
 - *Uses Gaussian approach to define clusters and uses both mean and std deviation unlike K-Means which only uses means. Detects elliptical clusters*
- Agglomerative Hierarchical Clustering
 - *Progressive pairwise clustering until all are merge into one tree in a dendrogram. Not too sensitive to choice of coefficient.*

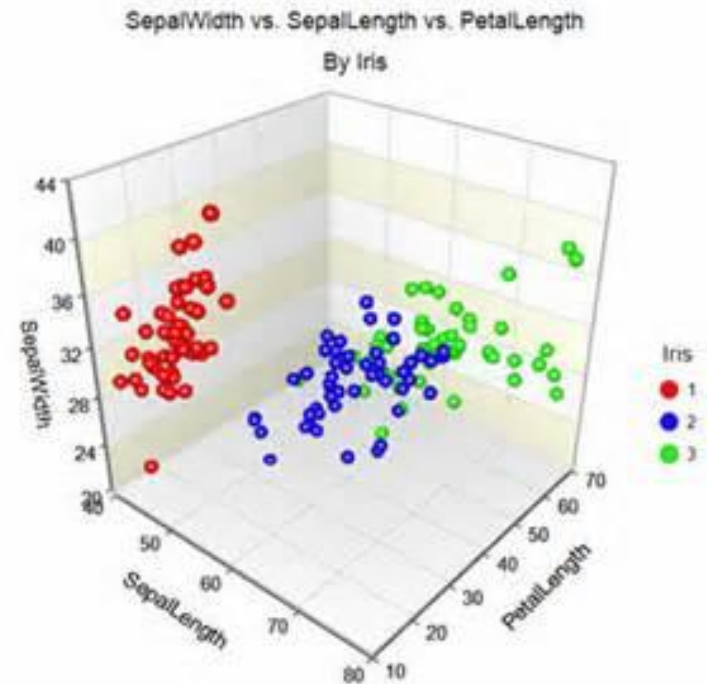
Cluster Analysis – Separating variables in n-dimensions

Visualization

2 dimensions



3 dimensions



4, 5,, n dimensions?

Cluster analysis requires:

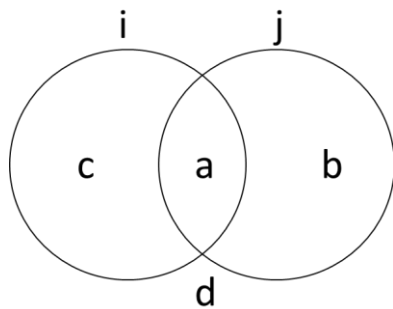
1. Measure of pairwise proximities between points
2. Grouping method

Proximity measures

Data

Measures of Similarity / Dissimilarity (Distance)

Binary
(presence/absence)



Continuous

Matching coefficient

Jaccard coefficient (1908)

Rogers & Tanimoto (1960)

Sneath & Sokal (1973)

Gower & Legendre (1986)

$$S_{ij} = (a + d) / (a + b + c + d)$$

$$S_{ij} = a / (a + b + c)$$

$$S_{ij} = (a + d) / [a + 2(b + c) + d]$$

$$S_{ij} = a / [a + 2(b + c)]$$

$$S_{ij} = (a + d) / [a + \frac{1}{2}(b + c) + d]$$

$$S_{ij} = a / [a + \frac{1}{2}(b + c)]$$

Euclidean Distance

Distance between vectors x & y

$$d(x, y) = \sqrt{\sum_i^n (x_i - y_i)^2}$$

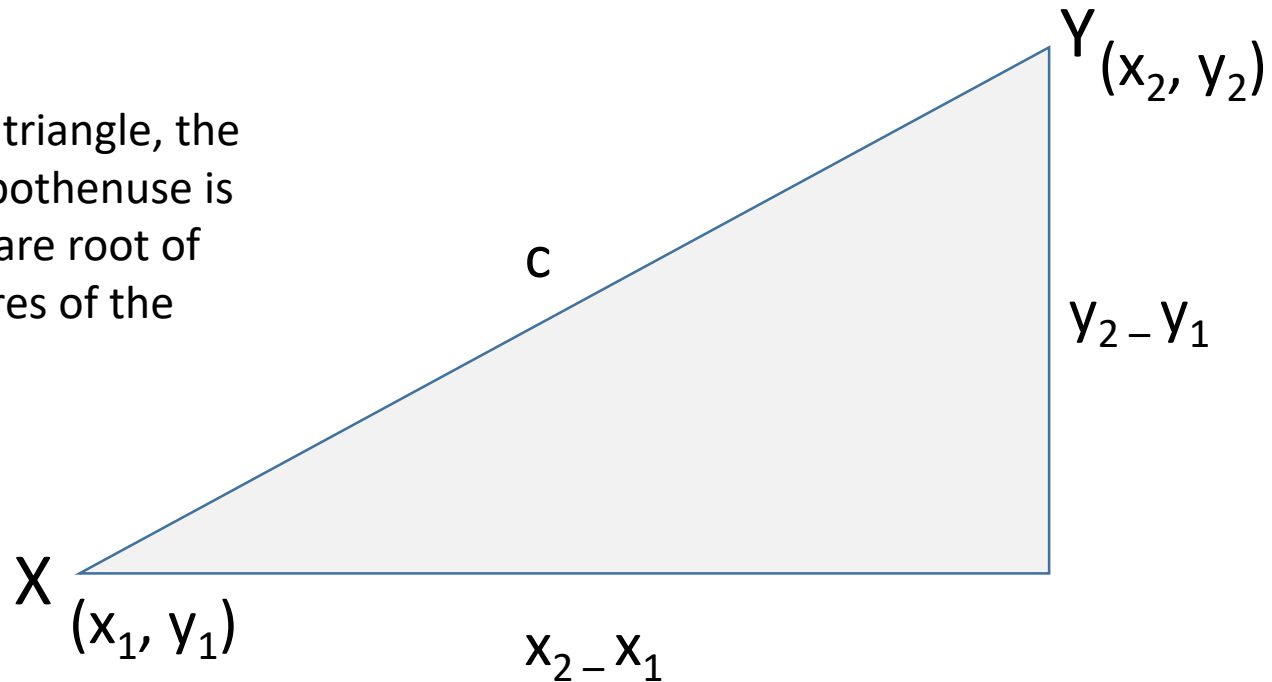
Canberra Distance

Distance between vectors u & v

$$d(u, v) = \sum_i \frac{|u_i - v_i|}{|u_i| + |v_i|}$$

Proximity measures - Euclidean Distance – Pythagoras's Theorem

In a right angled triangle, the length of the hypotenuse is equal to the square root of the sum of squares of the other 2 sides



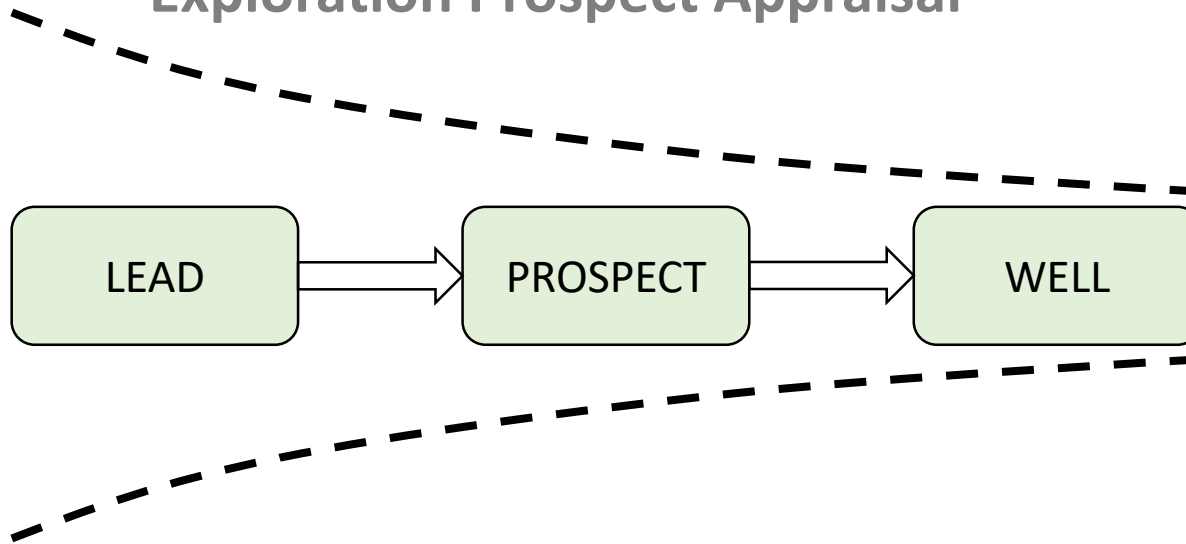
$$C = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

The Euclidean Distance $d(x, y) = \sqrt{\sum_i^n (x_i - y_i)^2} = C, n = 2$

Examples from Exploration data

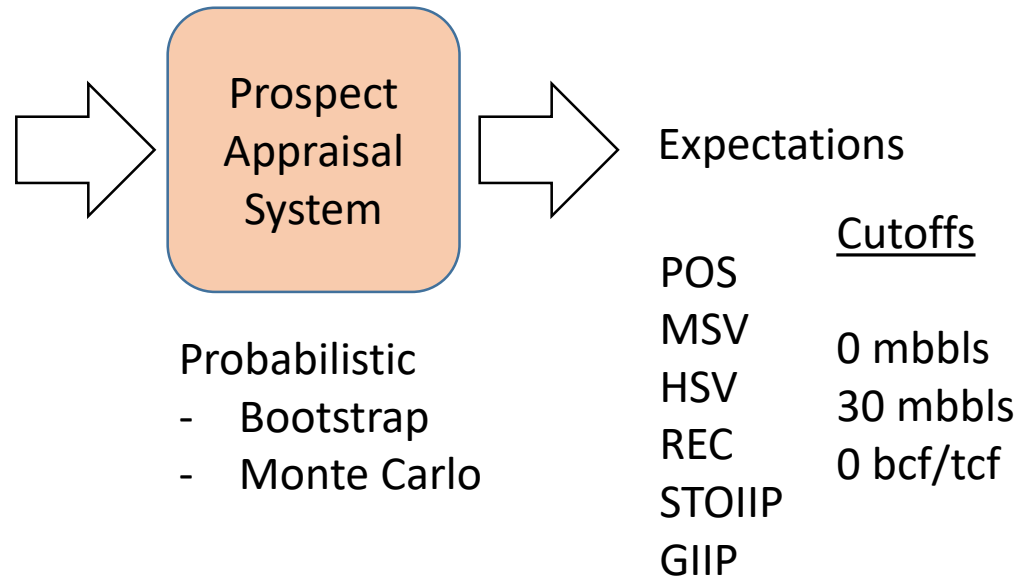
1. Prospect Appraisal – Expectation values
2. Well logs – Curve values
3. Micropaleontology – Foraminiferal assemblages

Exploration Prospect Appraisal



DATA

Seismic interpretation
Geological picks & zones
Paleontology (incl. palyn, nanno etc)
Lithology & Lithofacies
Environments of deposition
Temperature
etc



Precision-DM



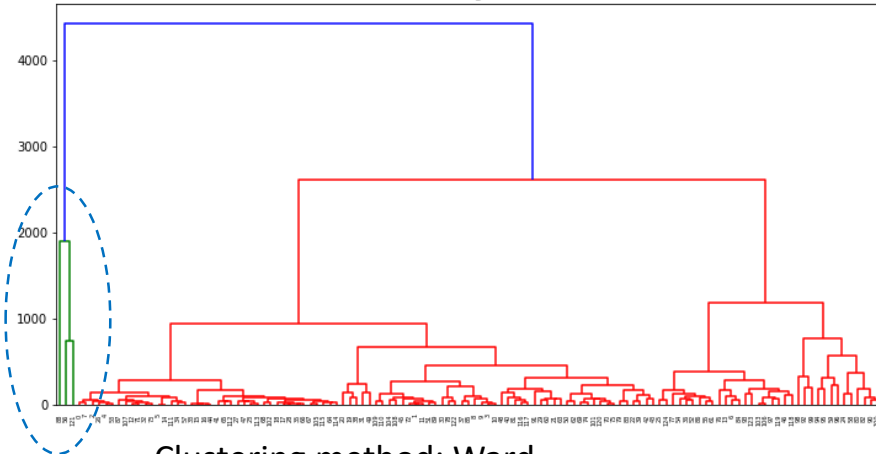
Exploration Prospect Appraisal – The DATA

OIL (0 mmbbls cutoff)					OIL (30 mmbbls cutoff)			GAS (0 bscf cutoff)			(values/POS)				
POS	MSV	HSV	Expectation		POS	MSV	HSV	POS	MSV	HSV	Expectation		MSV STOIIP	MSV GIIP	
			REC.	STOIIP							Rec.	GIIP			
80	6	10	5	24	1	21	0	96	79	133	76	122	30		127
64	11	26	7	23	10	38	60	64	25	57	16	27	36		42
68	11	23	8	31	15	29	38	80	41	90	33	55	46		69
85	5	9	4	27	0	0	0	85	15	32	13	25	32		29
72	7	16	5	22	6	29	40	80	27	64	22	36	31		45
78	3	6	2	11	0	0	0	87	13	30	11	18	14		21
80	4	8	3	11	0	0	0	99	29	49	29	49	14		49
81	11	22	9	43	18	28	36	90	55	114	50	82	53		91
26	8	19	2	10	4	29	36	29	35	75	10	16	38		55
65	4	6	2	12	0	0	0	72	34	59	24	34	18		47
80	2	2	1	5	0	0	0	92	6	12	6	9	6		10
85	22	41	18	73	40	36	52	95	113	219	107	184	86		194
48	2	4	1	5	0	0	0	80	18	33	14	29	10		36
48	2	4	1	5	0	0	0	80	18	33	14	29	10		36
90	18	37	16	76	29	37	56	99	53	109	52	88	84		89
84	20	48	17	81	29	47	75	94	57	135	54	92	96		98
81	11	21	9	37	12	26	31	83	61	110	51	91	46		110
81	11	21	9	37	12	26	31	83	61	110	51	91	46		110
80	12	24	9	46	16	28	37	90	61	125	55	92	58		102
80	12	24	9	46	16	28	37	90	61	125	55	92	58		102
67	6	11	4	17	1	27	34	80	29	61	23	36	25		45

The purpose: Exploring 'natural' groups of prospects may trigger ideas

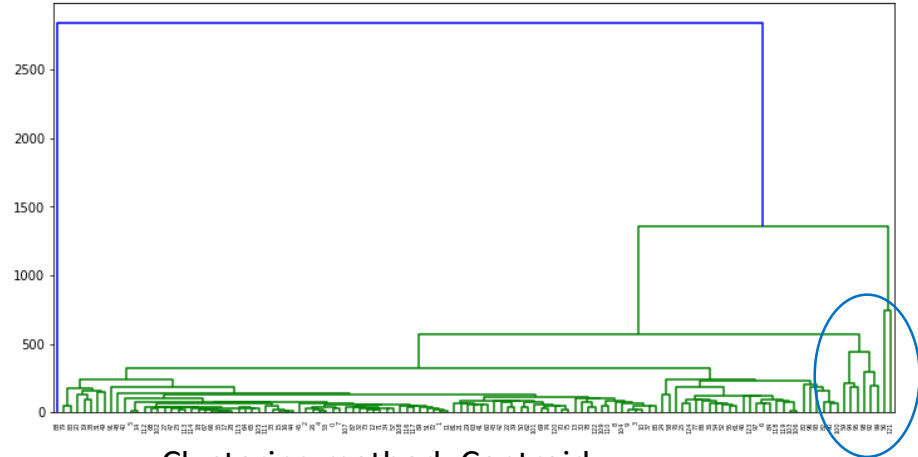
Exploration Prospect Appraisal - Clustering

Customer Dendograms - Ward's



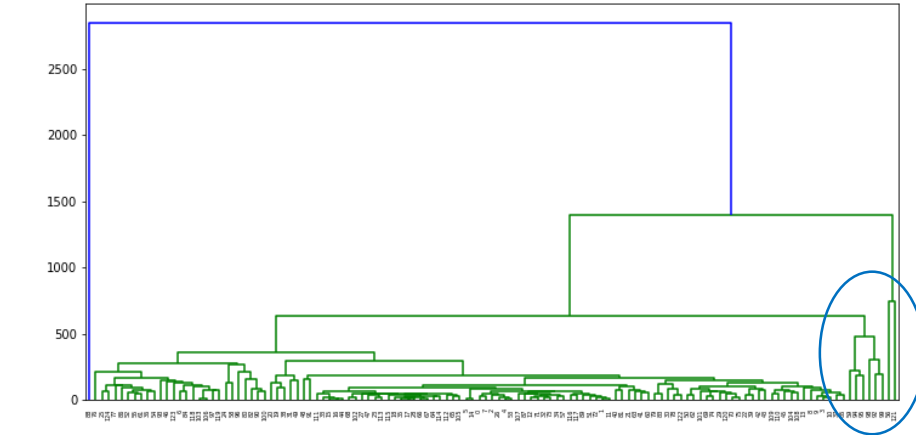
Clustering method: Ward
Coefficient: Squared Euclidean Distance

Customer Dendograms - Centroid



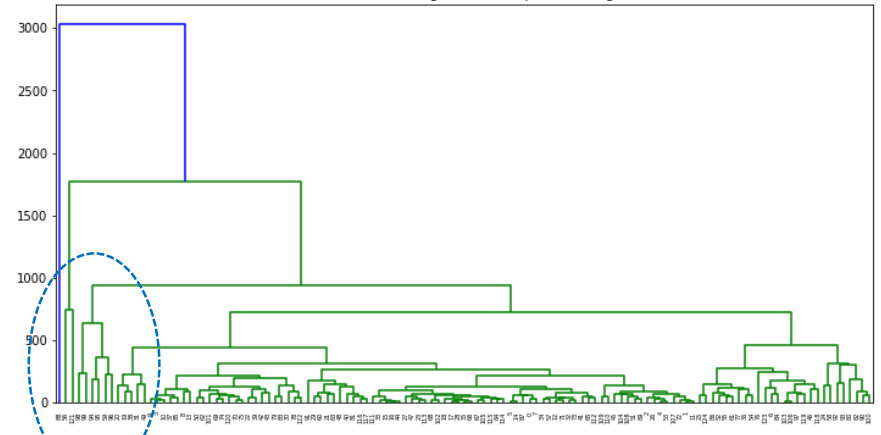
Clustering method: Centroid
Coefficient: Squared Euclidean Distance

Customer Dendograms - Average Linkage



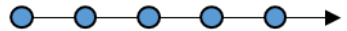
Clustering method: Average Linkage
Coefficient: Squared Euclidean Distance

Customer Dendograms - Complete Linkage



Clustering method: Complete Linkage
Coefficient: Squared Euclidean Distance

Precision-DM

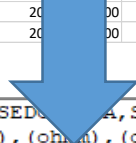


Cluster analysis using Spyder / Anaconda
Scipy.cluster.hierarchy.dendrogram

1. **Not very distinct clusters**
2. **Review data to remove non-discriminatory data**
3. **Rerun and review**

Well Curves – The DATA

Depth (ft)	SGRC (api)	SGRA (api)	SGRB (api)	SEXP (ohmm)	SESP (ohmm)	SEMP (ohmm)	SEDP (ohmm)	SEXC (ohmm)	SESC (ohmm)	SEMC (ohmm)	SEDC (ohmm)	SEDA (ohmm)	STEM (degF)	SDDE (ptpf)	SPLF (v/v)	SNNA (cp30)	SNFA (cp30)	SBDC (g/cc)	SCOR (g/cc)	SBD2 (g/cc)	SCO2 (g/cc)	SNBD (g/cc)	SFBD (g/cc)	SNPE (b/e)	SHSI (in)
1	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
10291	-999.25	-999.25	-999.25	0.06	0.06	120.34	975	0.09	0.09	36.32	194.42	194.42	142.46	-999.25	0.5	2440	475	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10291.5	-999.25	-999.25	-999.25	0.06	0.06	105.39	981.11	0.09	0.09	34.45	193.68	193.68	142.6	-999.25	0.5	2445	475	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10292	-999.25	-999.25	-999.25	0.06	0.06	84.5	986.24	0.09	0.09	31.12	191.57	191.57	142.77	-999.25	0.5	2457	474	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10292.5	-999.25	-999.25	-999.25	0.06	0.06	52.02	952.05	0.09	0.09	28.88	188.31	188.31	142.95	-999.25	0.5	2467	472	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10293	-999.25	-999.25	-999.25	0.06	0.06	32.12	927.16	0.09	0.09	28.85	186.63	186.63	143.16	-999.25	0.5	2470	472	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10293.5	-999.25	-999.25	-999.25	0.06	0.06	27.58	972.77	0.09	0.09	26.99	187.16	187.16	143.84	-999.25	0.5	2470	472	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10294	-999.25	-999.25	-999.25	0.06	0.06	31.96	1047.71	0.09	0.09	21.46	188.23	188.23	144.35	-999.25	0.49	2475	476	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25
10294.5	-999.25	-999.25	-999.25	0.06	0.06	64.08	1005.84	0.09	0.09	17.79	190.26	190.26	144.8	-999.25	0.49	2475	482	-999.25	-999.25	-999.25	-999.25	-999.25	-999.25	11.34	-999.25
10295	-999.25	-999.25	-999.25	0.06	0.06	125.01	886.83	0.09	0.09	13.62	192.59	192.59	145.28	5.66	0.48	2471	487	2.24	-0.29	-999.25	-999.25	-999.25	2.52	11.31	8.5
10295.5	-999.25	-999.25	-999.25	0.06	0.06	241.79	848.52	0.09	0.09	10.03	194.6	194.6	145.93	32.03	0.48	2466	490	2.23	-0.29	-999.25	-999.25	-999.25	2.52	11.32	8.5
10296	-999.25	-999.25	-999.25	0.06	0.06	480.27	976.85	0.09	0.09	5.39	200	200	146.32	51.08	0.48	2465	491	2.23	-0.29	-999.25	-999.25	-999.25	2.52	11.25	8.5
10296.5	-999.25	-999.25	-999.25	0.06	0.06	318.86	885.12	0.09	0.09	0.39	200	200	146.71	48.06	0.48	2462	492	2.23	-0.29	-999.25	-999.25	-999.25	2.52	11.22	8.5
10297	-999.25	-999.25	-999.25	0.06	0.06	188.62	966.88	0.09	0.09	0.45	200	200	147.06	63.25	0.48	2462	494	2.23	-0.29	-999.25	-999.25	-999.25	2.52	11.19	8.5
10297.5	-999.25	-999.25	-999.25	0.06	0.06	110.06	1315.63	0.09	0.09	0.36	200	200	147.62	82.68	0.48	2463	495	2.22	-0.29	-999.25	-999.25	-999.25	2.52	11.15	8.5
10298	-999.25	-999.25	-999.25	0.06	0.06	71.02	1518.89	0.09	0.09	0.32	200	200	147.99	46.49	0.48	2465	498	2.22	-0.3	-999.25	-999.25	-999.25	2.52	11.09	8.5
10298.5	-999.25	-999.25	-999.25	0.06	0.06	46.32	1565.17	0.09	0.09	0.29	200	200	148.39	26.48	0.47	2467	499	2.22	-0.3	-999.25	-999.25	-999.25	2.51	11.07	8.5

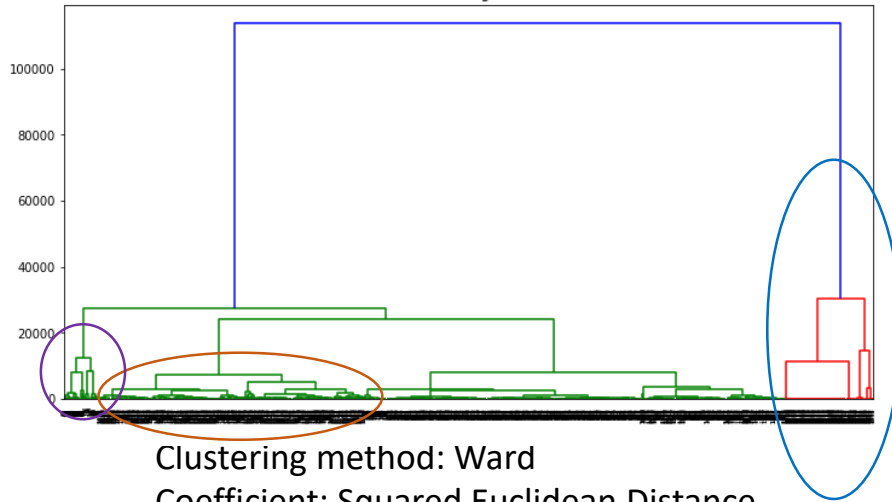


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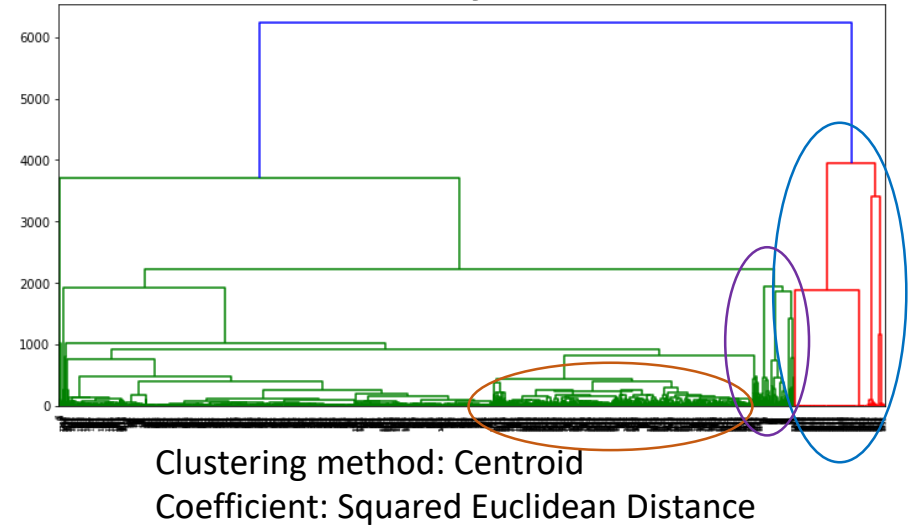
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(ft),(api),(api),(api),(ohmm),(ohmm),(ohmm),(ohmm),(ohmm),(ohmm),(ohmm),(ohmm),(degF),(ptpf),(v/v),(cp30),(cp30),(g/cc),(g/cc),
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10292,-999.25,-999.25,-999.25,0.06,0.06,84.5,986.24,0.09,0.09,31.12,191.57,191.57,142.77,-999.25,0.5,2457,474,-999.25,-999.25,-999.25
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Well Curves – Clustering

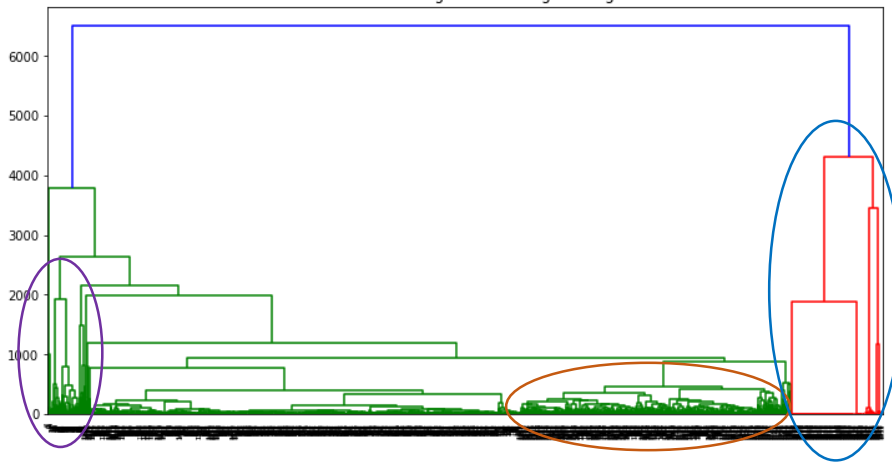
Customer Dendograms - Ward



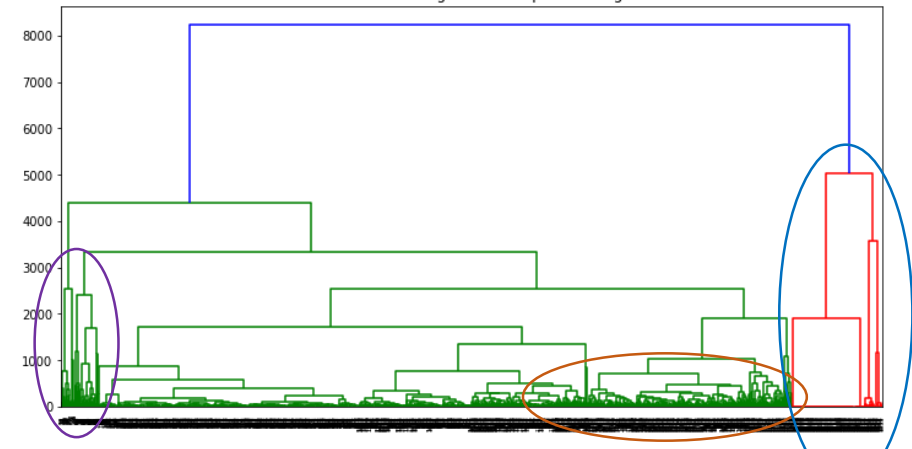
Customer Dendograms - Centroid



Customer Dendograms - Average Linkage



Customer Dendograms - Complete Linkage



Precision-DM

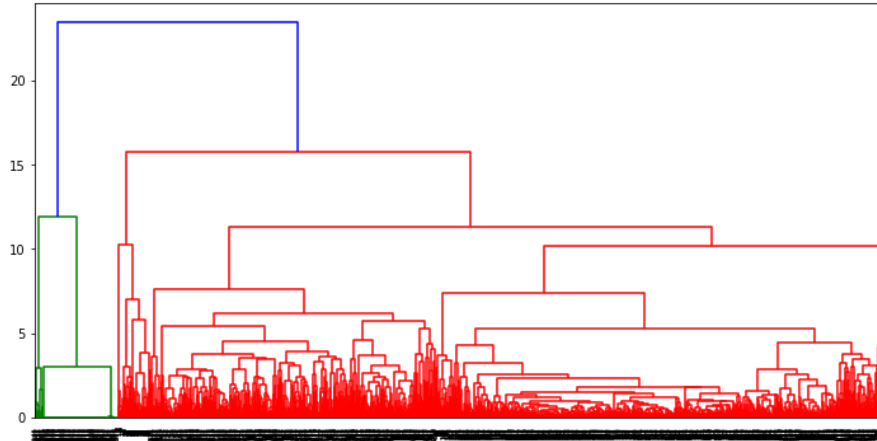


Cluster analysis using Spyder / Anaconda
Scipy.cluster.hierarchy.dendrogram

1. Some distinct clusters, majority of points are mixed
2. Review data to remove non-discriminatory data
3. Investigate end points. Rerun and review

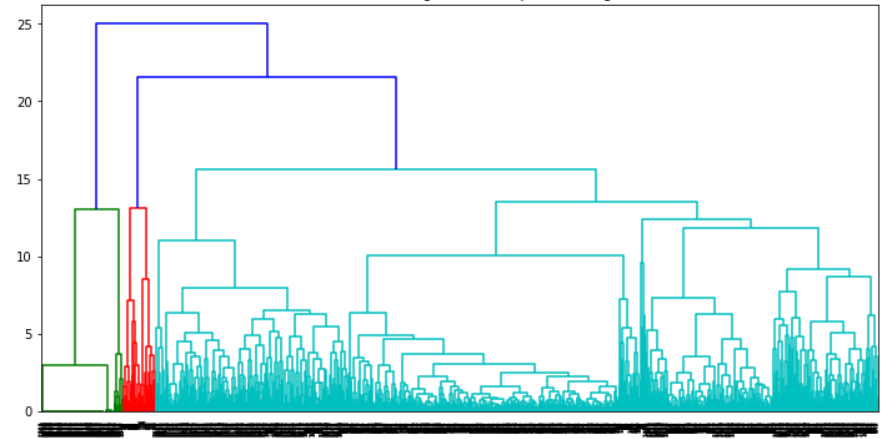
Well Curves – Change of coefficient

Customer Dendograms - Average Linkage



Clustering method: Average Linkage
Coefficient: Canberra

Customer Dendograms - Complete Linkage



Clustering method: Complete Linkage
Coefficient: Canberra

Precision-DM



Cluster analysis using Spyder / Anaconda
`Scipy.cluster.hierarchy.dendrogram`

1. More distinct clusters, easier to differentiate
2. Investigate groups for significance
3. Review data for noise

Micropaleontology



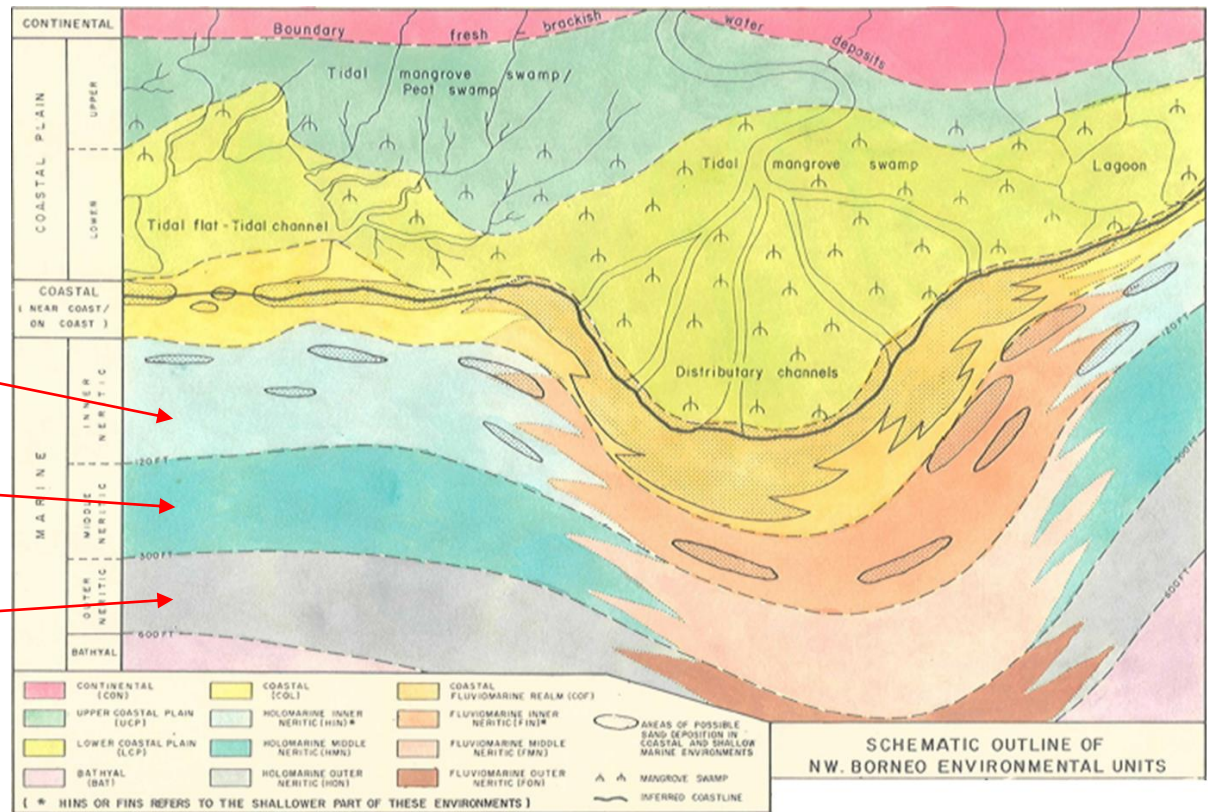
Benthonic Foraminifera – Protozoa. Live(d) on the sea bottom. Size ~ 200-2000 microns
Best viewed with binocular microscope at 25x – 80x magnification

North West Borneo Environmental Scheme (Shell, 1970s)

Holomarine Inner Neritic
0 – 40m water depth

Holomarine Middle Neritic
40 – 100m water depth

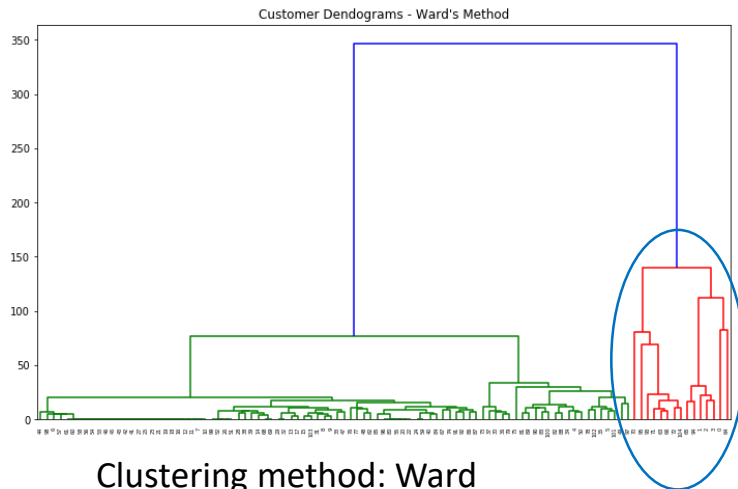
Holomarine Middle Neritic
100 – 200m water depth



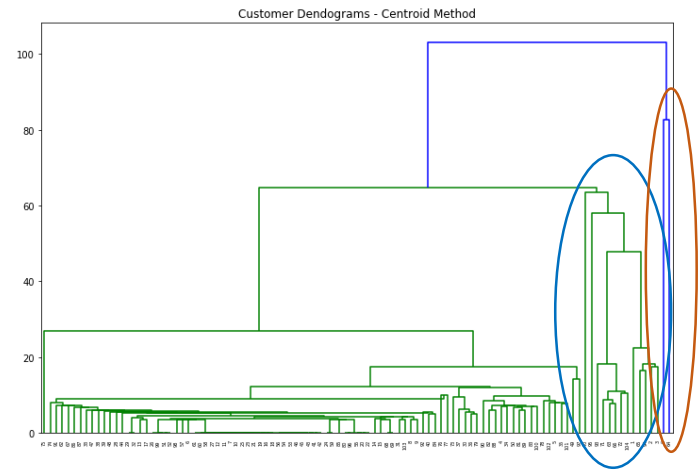
Micropaleontology – The DATA

[illegible][illegible]

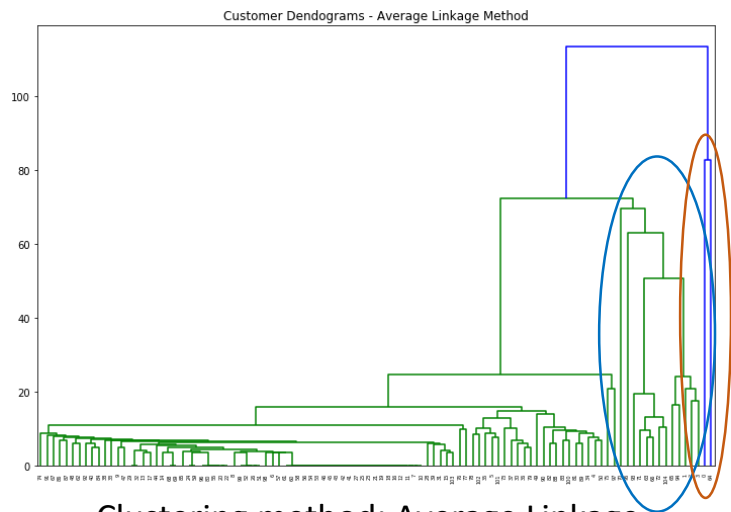
Micropaleontology – Well foraminiferal samples



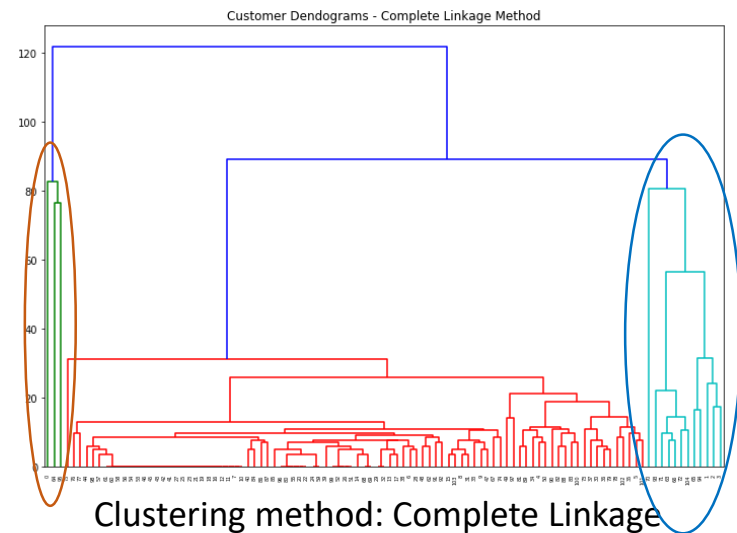
Clustering method: Ward
Coefficient: Squared Euclidean Distance



Clustering method: Centroid
Coefficient: Squared Euclidean Distance

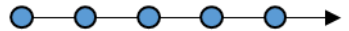


Clustering method: Average Linkage
Coefficient: Squared Euclidean Distance



Clustering method: Complete Linkage
Coefficient: Squared Euclidean Distance

Precision-DM



Cluster analysis using Spyder / Anaconda
Scipy.cluster.hierarchy.dendrogram

1. Some distinct clusters, mostly mixed
2. Investigate groups for significance
3. Review data for noise

Data Science opportunities – Paleoenvironmental reconstruction

Stratigraphy

- Litho, bio, chrono
- Sea level changes
- flooding surfaces

Sedimentary facies

- types
- characteristics
- bedding, dips etc
- log shape interpretation

Seismic

- seismic features (seismostrat)
- traces
- Checkshots
- time-depth curve
- Vertical seismic profiling (VSP)

Structural

- faults
- uplifts
- eustatic
- erosion
- missing sections

Well Logs

- Gamma ray
- Sonic
- Density
- Neutron
- Resistivities
- Caliper

Minerals

- glauconite
- siderite
- pyrite
- mica

Paleontology

- benthics
- planktonics
- larger forams
- nannofossils
- palynology
- ostracods
- trace fossils



Data Science opportunities— Source Rocks

Pressure

- Spot readings
- Trends

Well Logs

- Gamma ray
- Sonic
- Density
- Resistivities
- Caliper

Sedimentary facies

- types
- characteristics
- bedding, dips etc
- log shape interpretation

Rock properties

- Porosity
- Permeability
- Diagenesis

Temperature

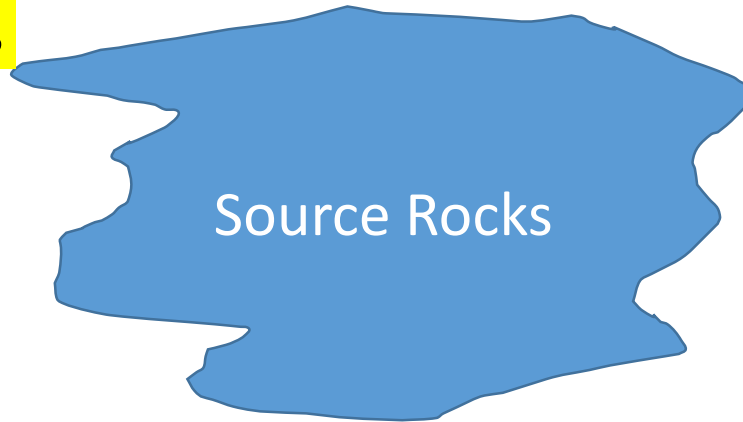
- Sample readings
- Gradients

Macerals

- Organic type (Lip. vs Vit.)
- Kitchen area
- Migration paths
- Maturity levels (DOM, VR/E)

Surrounding wells

- well data
- Source rock distribution patterns
- maps & trends



Burial History

- Sedimentation rates
- Sediment types
- Missing sections
- Palinspastic reconstruction

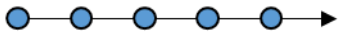
Computer simulation

- Methods (eg Migration Models)
- Probabilistic vs deterministic

Paleontology

- benthics
- planktonics
- larger forams
- nannofossils
- palynology
- ostracods

Precision-**DM**



Data Science opportunities— Prospect appraisal

Temperature

- Sample readings
- Gradients

Pressure

- Spot readings
- Trends

Analogues

- local comparators
- regional
- global

Sedimentary facies

- Sediment types
- Characteristics
- Bedding, dips etc
- Log shape interpretation

Structural

- faults
- closures
- seals

Surrounding wells

- Well data
- Correlation
- Maps & trends



Burial History

- Sedimentation rates
- Sediment types
- Missing sections
- Palinspastic reconstruction

Rock properties

- Porosity
- Permeability
- Diagenesis

Well Logs

- Gamma ray
- Sonic
- Density
- Neutron
- Resistivities
- Caliper

Computer simulation

- Methods (eg Monte carlo)
- Probablistic vs deterministic

Source Rocks

- Type (lip. vs vit.)
- Kitchen area
- Maturity

Paleontology

- benthics
- planktonics
- larger forams
- nannofossils
- palynology
- ostracods

Conclusions

- Machine learning is not a black box
- Understand the ML workflow components, behaviors and limitations
- Look at the DATA
- Give importance to feature selection & feature extraction
- Look at the results
- Look at the DATA again

Questions