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INTRODUCTION TO MACHINE LEARNING

DIT 45100

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Unsupervised Machine Learning

Agenda

- Big Idea
- Fundamentals
- Standard Approach: The k-Means Clustering Algorithm
- Extensions and Variations
- Summary

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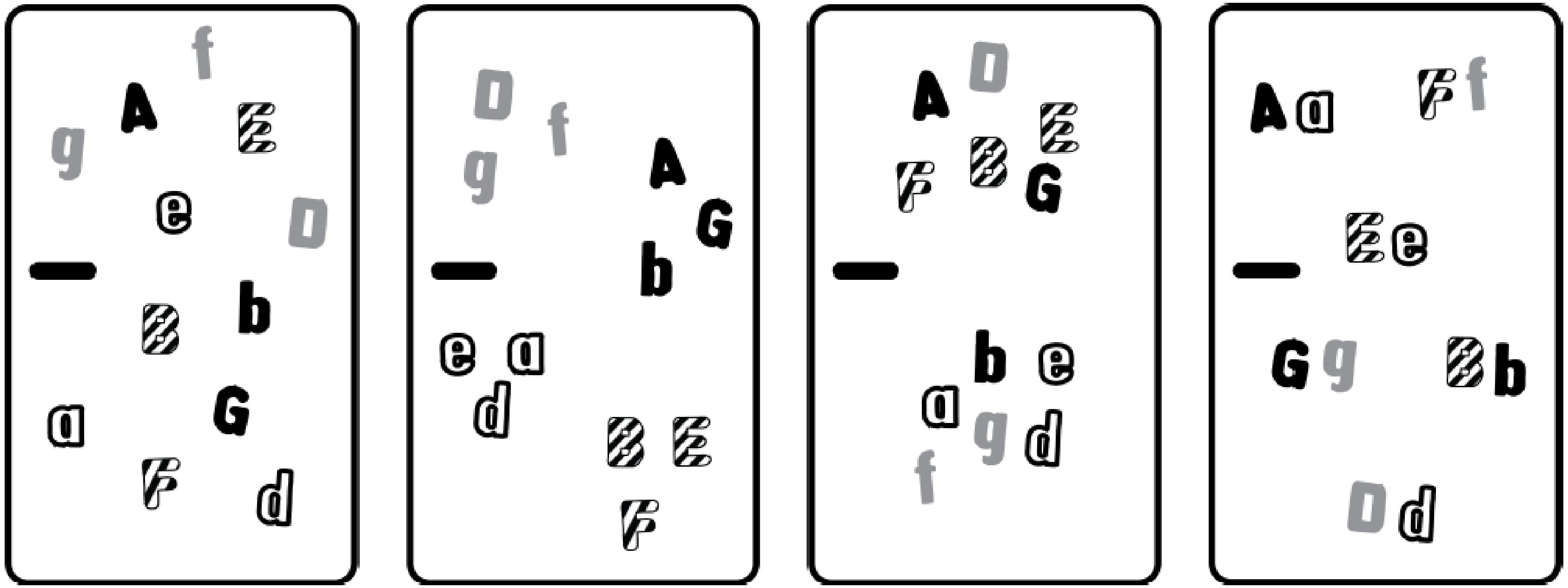
Big Idea



(a) The fridge (b) Abigail (c) Andrew (d) Amalia

Figure 1: The three different arrangements of the magnetic letters made by the Murphy children on the Murphy family refrigerator.

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Fundamentals

Unsupervised ML

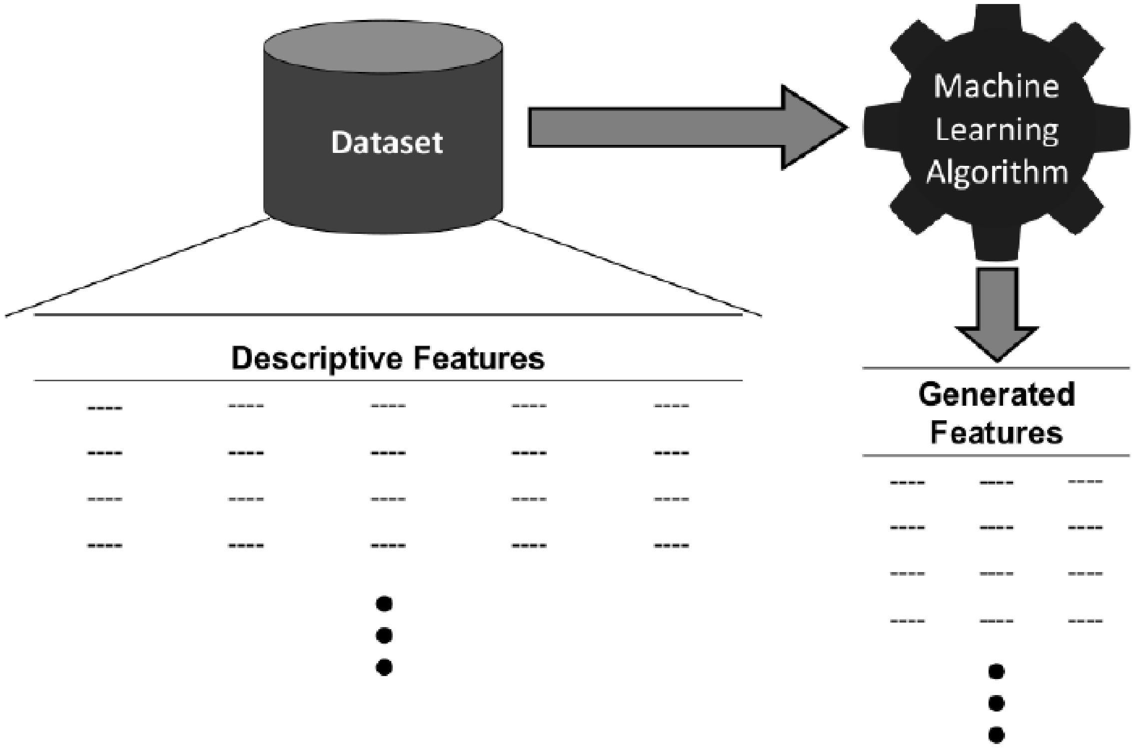

Figure 2: Unsupervised machine learning as a single-step process.

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Standard Approach: The k-Means Clustering Algorithm

K-Means Clustering

$$\sum_{i=1}^{n} \min_{\mathbf{c}_1,\ldots,\mathbf{c}_k} Dist(\mathbf{d}_i, \mathbf{c}_j) \qquad (1)$$

K-Means Clustering Algorithm

Require: a dataset $\mathcal{D}$ containing n training instances, $\mathbf{d}_1, \ldots, \mathbf{d}_n$
Require: the number of clusters to find k
Require: a distance measure, $Dist$, to compare instances to cluster centroids

1: Select k random cluster centroids, $\mathbf{c}_1$ to $\mathbf{c}_k$, each defined by values for each descriptive feature, $\mathbf{c}_i =< \mathbf{c}_i[1], \ldots, \mathbf{c}_i[m] >$
2: **repeat**
3: calculate the distance of each instance, $\mathbf{d}_i$, to each cluster centroid, $\mathbf{c}_1$ to $\mathbf{c}_k$, using $Dist$
4: assign each instance, $\mathbf{d}_i$, to belong to the cluster, $\mathcal{C}_i$, to whose cluster centroid, $\mathbf{c}_i$, it is closest
5: update each cluster centroid, $\mathbf{c}_i$, to the average of the descriptive feature values of the instances that belong to cluster $\mathcal{C}_i$
6: **until** no cluster reassignments are performed during an iteration

Table 1: A dataset of mobile phone customers described by their average monthly data (DATA USAGE) and call (CALL VOLUME) usage. Details of the first two iterations of the k-means clustering algorithm are also shown.

ID	DATA USAGE	CALL VOLUME	Cluster Distances Iter. 1			Iter. 1	Cluster Distances Iter.	
			$Dist(\mathbf{d}_i, \mathbf{c}_1)$	$Dist(\mathbf{d}_i, \mathbf{c}_2)$	$Dist(\mathbf{d}_i, \mathbf{c}_3)$	Cluster	$Dist(\mathbf{d}_i, \mathbf{c}_1)$	$Dist(\mathbf{d}_i, \mathbf{c}_2)$
1	-0.9531	-0.3107	0.2341	0.9198	0.6193	$\mathcal{C}_1$	0.4498	1.9014
2	-1.1670	-0.7060	0.5770	0.6108	0.9309	$\mathcal{C}_1$	0.87	2.0554
3	-1.2329	-0.4188	0.3137	0.8945	0.6388	$\mathcal{C}_1$	0.7464	2.152
4	1.0684	-0.4560	2.1972	2.06	2.438	$\mathcal{C}_2$	1.6857	0.3813
5	-1.1104	0.1090	0.2415	1.3594	0.1973	$\mathcal{C}_3$	0.5669	2.1905
6	-0.8431	0.1811	0.4084	1.405	0.4329	$\mathcal{C}_1$	0.3694	1.9842
7	-0.3666	0.6905	1.1055	1.9728	1.0231	$\mathcal{C}_3$	0.7885	1.9406
8	0.9285	-0.2168	2.0351	2.0378	2.2455	$\mathcal{C}_1$	1.5083	0.5759
9	1.1175	-0.6028	2.2715	2.0566	2.529	$\mathcal{C}_2$	1.772	0.298
10	0.8404	-1.0450	2.1486	1.693	2.4636	$\mathcal{C}_2$	1.7165	0.258
11	-1.005	-0.0337	0.1404	1.2012	0.3692	$\mathcal{C}_1$	0.4339	2.0376
12	0.2410	0.7360	1.6017	2.2398	1.6013	$\mathcal{C}_3$	1.1457	1.6581
13	0.2021	0.4364	1.4253	1.9619	1.4925	$\mathcal{C}_1$	0.9259	1.4055
14	0.2153	0.8360	1.6372	2.3159	1.6125	$\mathcal{C}_3$	1.2012	1.7602
15	0.8770	-0.2459	1.985	1.9787	2.201	$\mathcal{C}_2$	1.4603	0.5454
16	-0.0345	1.0502	1.595	2.4136	1.4929	$\mathcal{C}_3$	1.2433	2.0589
17	0.8785	-1.3601	2.3325	1.727	2.6698	$\mathcal{C}_2$	1.9413	0.569
18	0.9164	-0.8517	2.1454	1.7984	2.4383	$\mathcal{C}_2$	1.6815	0.0674
19	-1.0423	0.1193	0.2593	1.3579	0.2525	$\mathcal{C}_3$	0.5065	2.133
20	-0.7426	0.0119	0.3899	1.2399	0.5706	$\mathcal{C}_1$	0.1889	1.8164
21	0.6259	-1.1834	2.0248	1.4696	2.3616	$\mathcal{C}_2$	1.6355	0.4709
22	0.7684	-0.5844	1.927	1.7338	2.195	$\mathcal{C}_2$	1.4362	0.2382
23	-0.2596	0.7450	1.2183	2.0535	1.1432	$\mathcal{C}_3$	0.8736	1.9167
24	-0.3414	0.4215	0.9432	1.7202	0.9548	$\mathcal{C}_1$	0.5437	1.7259

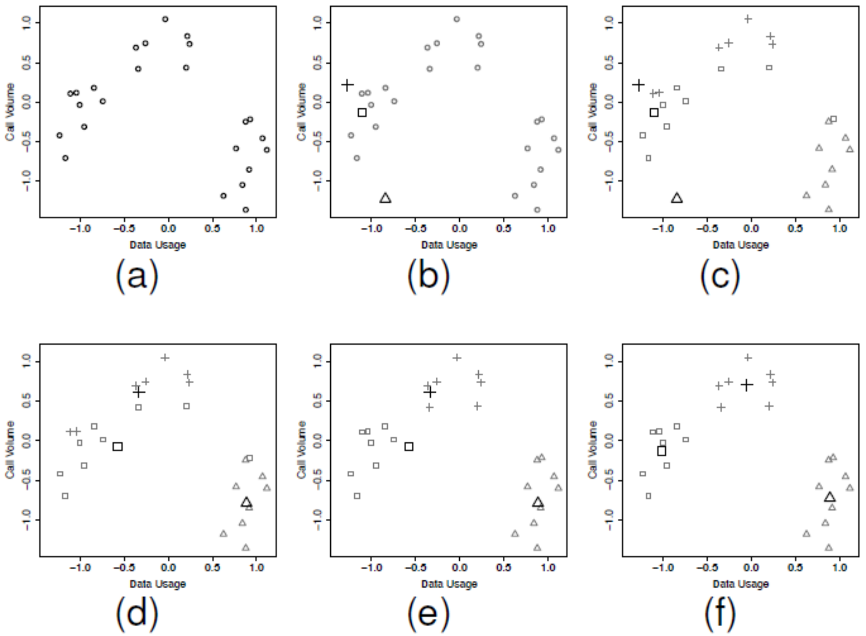

Figure 3: (a) A plot of the mobile phone customer dataset given in Table 1[10]. (b)–(f) The progress of the *k*-means clustering algorithm, working on the simple customer segmentation dataset. The large symbols represent cluster centroids, and the smaller symbols represent cluster assignments.

A Worked Example

$$
\begin{aligned}
\mathbf{c}_1[\textsc{Data Usage}] &= (-0.9531 + -1.167 + -1.2329 + -0.8431 + 0.9285 \\
&\qquad + -1.005 + 0.2021 + -0.7426 + -0.3414)/9 \\
&= -0.5727 \\
\mathbf{c}_1[\textsc{Call Volume}] &= (-0.3107 + -0.706 + -0.4188 + 0.1811 + -0.2168 \\
&\qquad + -0.0337 + 0.4364 + 0.0119 + 0.4215)/9 \\
&= -0.0706
\end{aligned}
$$

A Worked Example

$$
\begin{aligned}
\mathcal{C}_1 &= \{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \mathbf{d}_5, \mathbf{d}_6, \mathbf{d}_{11}, \mathbf{d}_{19}, \mathbf{d}_{20}\} \\
\mathcal{C}_2 &= \{\mathbf{d}_4, \mathbf{d}_8, \mathbf{d}_9, \mathbf{d}_{10}, \mathbf{d}_{15}, \mathbf{d}_{17}, \mathbf{d}_{18}, \mathbf{d}_{21}, \mathbf{d}_{22}\} \\
\mathcal{C}_3 &= \{\mathbf{d}_7, \mathbf{d}_{12}, \mathbf{d}_{13}, \mathbf{d}_{14}, \mathbf{d}_{16}, \mathbf{d}_{23}, \mathbf{d}_{24}\}
\end{aligned}
$$

Extensions and Variations

Choosing Initial Cluster Centroids

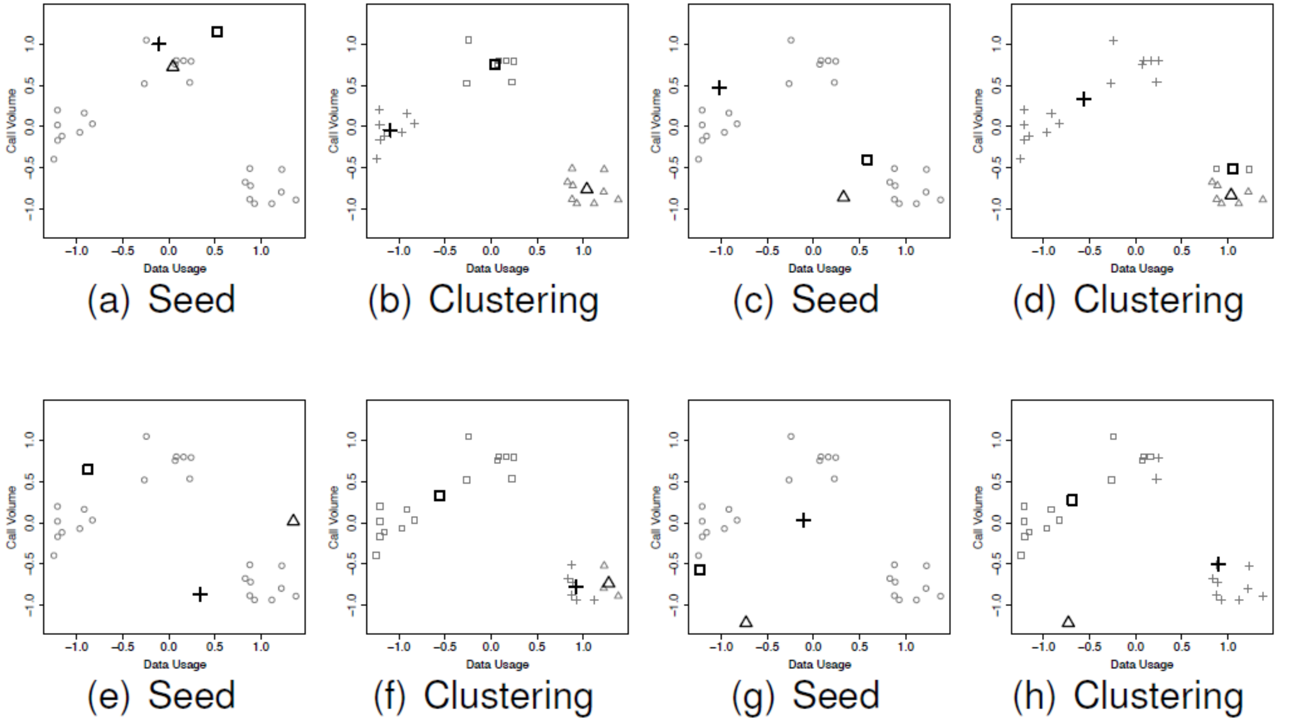

Figure 4: (a)–(h) Different clusterings (all with $k = 3$) that can be found for the mobile phone customer dataset given in Table 1[10] when different initial cluster centroids are used.

Choosing Initial Cluster Centroids

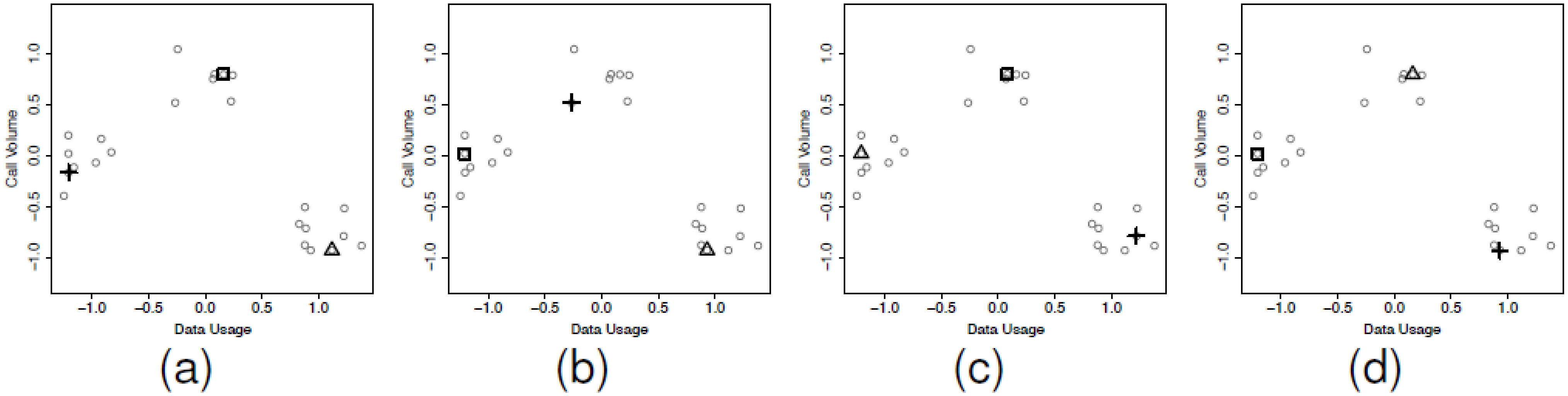

Figure 5: (a)–(d) Initial centroids chosen using the k-means++ approach (all with $k = 3$) for the mobile phone customer dataset given in Table 1[10].

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Evaluating Clustering

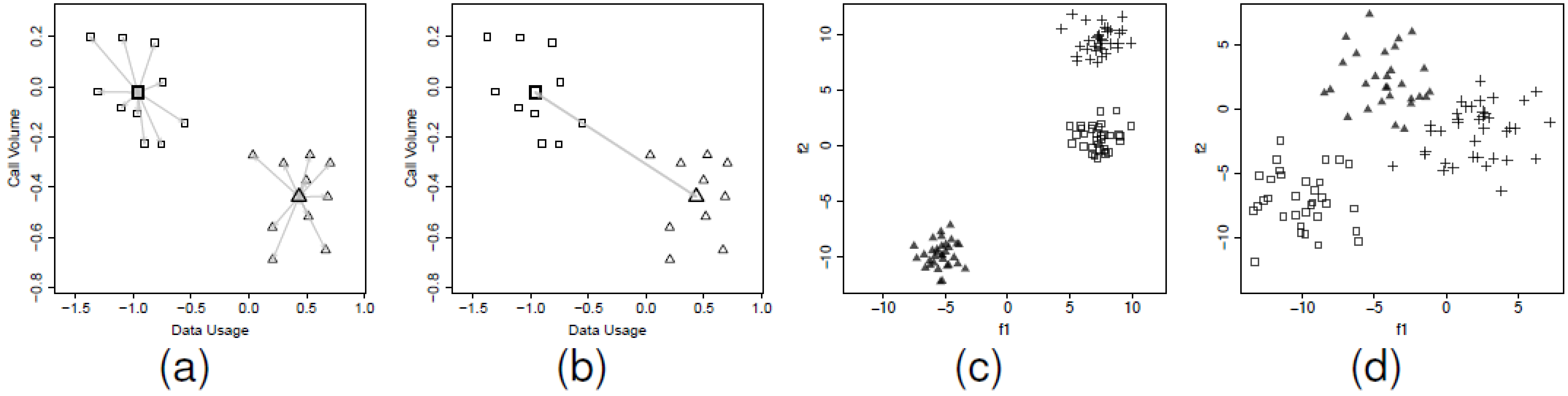

Figure 6: (a) Intra-cluster distance; (b) inter-cluster distance; (c) a *good* clustering; and (d) a *bad* clustering.

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Evaluating Clustering: Silhouette

$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))} \qquad (2)$$

Evaluating Clustering: Silhouette

$$
\begin{array}{cc}
 & \begin{array}{ccccccc} \mathbf{d}_2 & \mathbf{d}_3 & \mathbf{d}_5 & \mathbf{d}_6 & \mathbf{d}_{11} & \mathbf{d}_{19} & \mathbf{d}_{20} \end{array} \\
\mathbf{d}_1 & \left[\begin{array}{ccccccc} 0.45 & 0.30 & 0.45 & 0.50 & 0.28 & 0.44 & 0.39 \end{array} \right]
\end{array}
$$

$$
\begin{array}{cc}
 & \begin{array}{ccccccccc} \mathbf{d}_4 & \mathbf{d}_8 & \mathbf{d}_9 & \mathbf{d}_{10} & \mathbf{d}_{15} & \mathbf{d}_{17} & \mathbf{d}_{18} & \mathbf{d}_{21} & \mathbf{d}_{22} \end{array} \\
\mathbf{d}_1 & \left[\begin{array}{ccccccccc} 2.03 & 1.88 & 2.09 & 1.94 & 1.83 & 2.11 & 1.95 & 1.80 & 1.74 \end{array} \right]
\end{array}
$$

$$
\begin{array}{cc}
 & \begin{array}{ccccccc} \mathbf{d}_7 & \mathbf{d}_{12} & \mathbf{d}_{13} & \mathbf{d}_{14} & \mathbf{d}_{16} & \mathbf{d}_{23} & \mathbf{d}_{24} \end{array} \\
\mathbf{d}_1 & \left[\begin{array}{ccccccc} 1.16 & 1.59 & 1.38 & 1.64 & 1.64 & 1.26 & 0.95 \end{array} \right]
\end{array}
$$

Evaluating Clustering: Silhouette

$$\frac{1.3743 - 0.401}{max(0.401, 1.374)} = 0.7081$$

Evaluating Clustering: Silhouette

Pseudocode description of the algorithm for calculating the **silhouette** for internal cluster evaluation.

Require: a dataset $\mathcal{D}$ containing n training instances, $\mathbf{d}_1, \ldots, \mathbf{d}_n$
Require: a clustering $\mathcal{C}$ of dataset $\mathcal{D}$ into k clusters, $\mathcal{C}_1, \ldots, \mathcal{C}_k$
Require: a distance measure, $Dist$, to compare distances between instances

for each instance $\mathbf{d}_i$ in $\mathcal{D}$ **do**
 let $a(i)$ be the average distance between instance $\mathbf{d}_i$ and all of the other instances within the cluster to which $\mathbf{d}_i$ belongs, $\mathcal{C}_j$ (*average intra-cluster distance*)
 calculate the average distance between instance $\mathbf{d}_i$ and the members of each of the other clusters $\mathcal{C} \setminus \mathcal{C}_j$
 let $b(i)$ be the lowest average distance between instance $\mathbf{d}_i$ and any other cluster (*average inter-cluster distance*)
 calculate the silhouette index for $\mathbf{d}_i$ as

$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))} \quad (3)$$

end for
calculate final silhouette for the clustering as $s = \frac{1}{n}\sum_{i=1}^{n} s(i)$

Evaluating Clustering

Table 2: Calculating the silhouette for the final clustering of the mobile phone customer dataset (Table 1[10]) found using the *k*-means algorithm (with $k = 3$). The overall silhouette index value is 0.66.

ID	Cluster	Nearest Cluster	$a(i)$	$b(i)$	$s(i)$	ID	Cluster	Nearest Cluster	$a(i)$	$b(i)$	$s(i)$
1	$\mathcal{C}_1$	$\mathcal{C}_3$	0.401	1.374	0.708	13	$\mathcal{C}_3$	$\mathcal{C}_1$	0.5136	1.3592	0.6221
2	$\mathcal{C}_1$	$\mathcal{C}_3$	0.695	1.811	0.616	14	$\mathcal{C}_3$	$\mathcal{C}_1$	0.4349	1.5738	0.7236
3	$\mathcal{C}_1$	$\mathcal{C}_3$	0.503	1.644	0.694	15	$\mathcal{C}_2$	$\mathcal{C}_3$	0.5776	1.3480	0.5715
4	$\mathcal{C}_2$	$\mathcal{C}_3$	0.484	1.628	0.703	16	$\mathcal{C}_3$	$\mathcal{C}_1$	0.4955	1.5409	0.6784
5	$\mathcal{C}_1$	$\mathcal{C}_3$	0.387	1.232	0.686	17	$\mathcal{C}_2$	$\mathcal{C}_1$	0.7369	2.2757	0.6762
6	$\mathcal{C}_1$	$\mathcal{C}_3$	0.445	0.970	0.541	18	$\mathcal{C}_2$	$\mathcal{C}_3$	0.4312	1.8473	0.7666
7	$\mathcal{C}_3$	$\mathcal{C}_1$	0.452	1.056	0.572	19	$\mathcal{C}_1$	$\mathcal{C}_3$	0.3711	1.1682	0.6823
8	$\mathcal{C}_2$	$\mathcal{C}_3$	0.599	1.364	0.561	20	$\mathcal{C}_1$	$\mathcal{C}_3$	0.4334	1.0006	0.5669
9	$\mathcal{C}_2$	$\mathcal{C}_3$	0.470	1.768	0.734	21	$\mathcal{C}_2$	$\mathcal{C}_1$	0.6520	1.9710	0.6692
10	$\mathcal{C}_2$	$\mathcal{C}_3$	0.504	1.978	0.745	22	$\mathcal{C}_2$	$\mathcal{C}_3$	0.4504	1.5457	0.7086
11	$\mathcal{C}_1$	$\mathcal{C}_3$	0.327	1.223	0.732	23	$\mathcal{C}_3$	$\mathcal{C}_1$	0.3954	1.1654	0.6607
12	$\mathcal{C}_3$	$\mathcal{C}_1$	0.433	1.537	0.719	24	$\mathcal{C}_3$	$\mathcal{C}_1$	0.5339	0.8880	0.3988

Evaluating Clustering

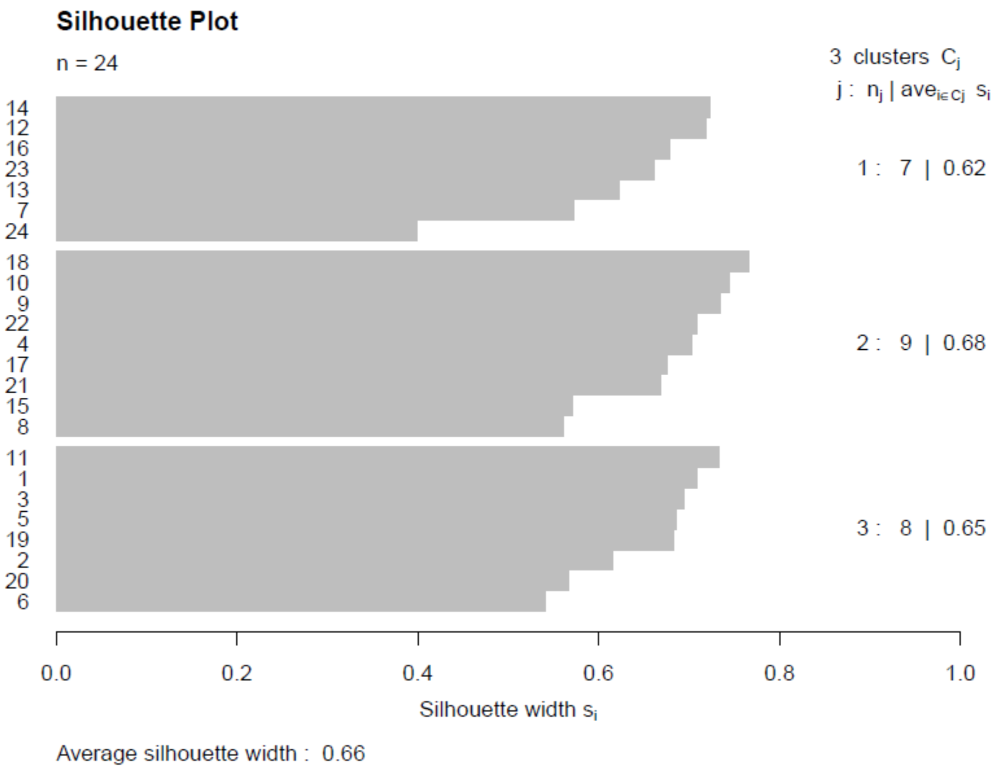

Figure 7: The silhouette plot for the final clustering of the mobile phone customer dataset (Table 1[10]) found using the *k*-means algorithm (with $k = 3$).

Understanding the Clustering Results

Table 3: Summary statistics for the three clusters found in the mobile phone customer dataset in Table 1[10] using *k*-means clustering ($k = 3$). Note, that the % missing and cardinality columns usually used are omitted here for legibility as these data quality issues will not arise in this simple example. They could be included when this approach is used on *real* datasets.

Feature	Cluster	Count	Min.	1^{st} Qrt.	Mean	Median	3^{rd} Qrt.	Max	Std. Dev.
DATA USAGE	$\mathcal{C}_1$	8	-1.2329	-1.1246	-1.0121	-1.0237	-0.9256	-0.7426	0.1639
	$\mathcal{C}_2$	9	0.6259	0.8404	0.8912	0.8785	0.9285	1.1175	0.1471
	$\mathcal{C}_3$	7	-0.3666	-0.3005	-0.0491	-0.0345	0.2087	0.241	0.2732
CALL VOLUME	$\mathcal{C}_1$	8	-0.7060	-0.3377	-0.1310	-0.0109	0.1116	0.1811	0.3147
	$\mathcal{C}_2$	9	-1.3601	-1.0450	-0.7273	-0.6028	-0.4560	-0.2168	0.4072
	$\mathcal{C}_3$	7	0.4215	0.5635	0.7022	0.7360	0.7905	1.0502	0.2204

Understanding the Clustering Results

Table 4: Information gain for each descriptive feature as a predictor of membership of each cluster based on the clustering of the mobile phone customer dataset in Table 1[10] found using k-means clustering ($k = 3$).

$\mathcal{C}_1$		$\mathcal{C}_2$		$\mathcal{C}_3$	
Feature	Info. Gain	Feature	Info. Gain	Feature	Info. Gain
DATA.USAGE	0.9183	DATA.USAGE	0.9544	CALL.VOLUME	0.8709
CALL.VOLUME	0.2117	CALL.VOLUME	0.5488	DATA.USAGE	0.2479

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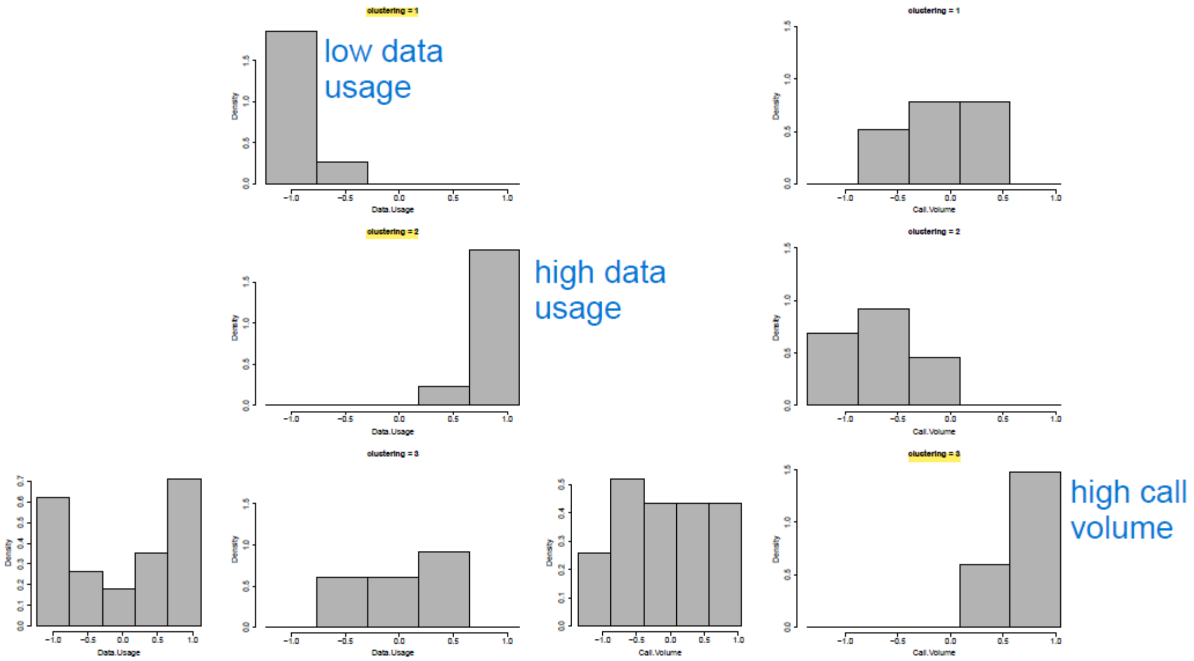
Understanding the Clustering Results



(a) Data Usage (b) Call Volume

Figure 9: (a)–(b) Visualizations of the distributions of the descriptive features in the mobile phone customer dataset in Table 1[10] across the complete dataset, and divided by the clustering found using k-means clustering ($k = 3$).

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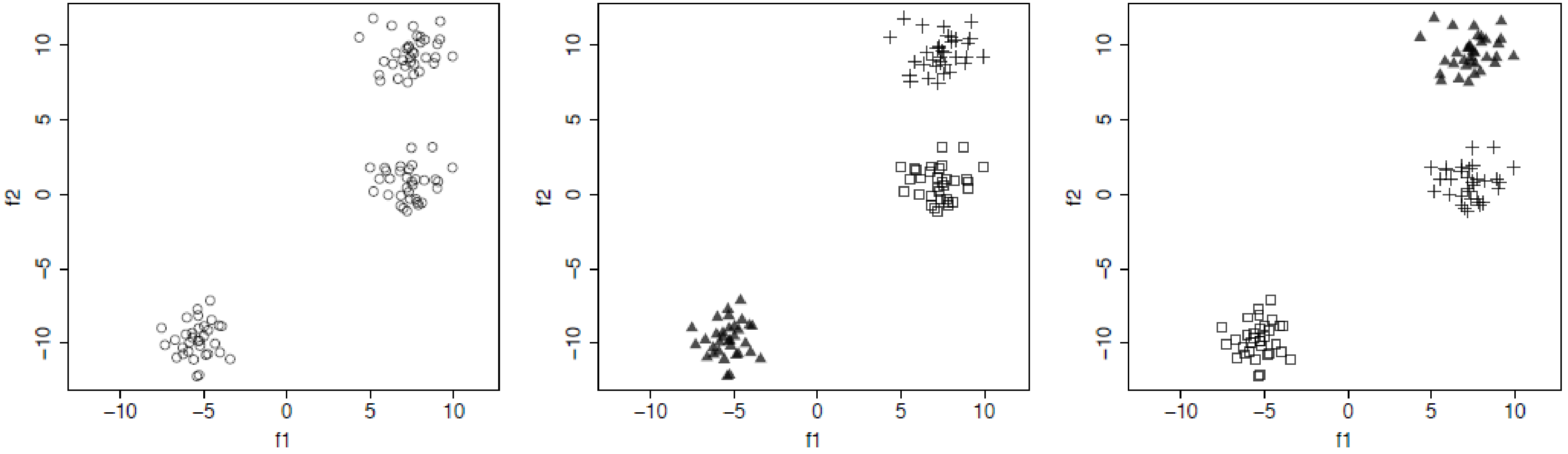
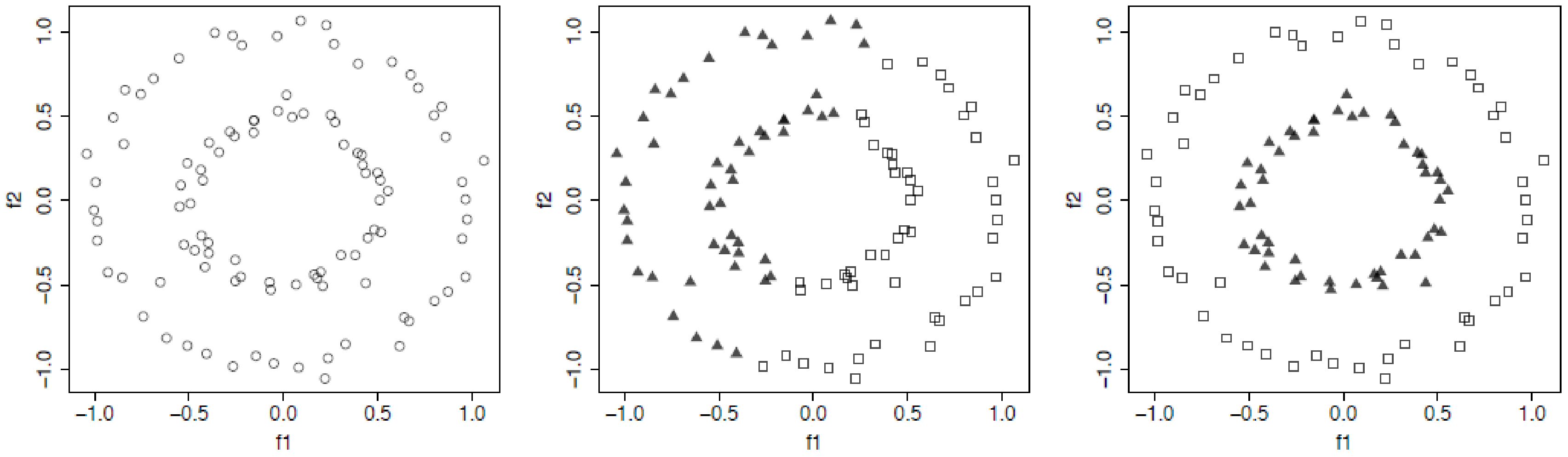
Agglomerative Hierarchical Clustering

AHC



(a) Blobs Dataset (b) k-means (c) AHC

Figure 10: (a)–(i) A plot of the *blobs*, *circles*, and *half-moons* datasets and the clusterings achieved by the *k*-means clustering and agglomerative hierarchical clustering algorithms (where k is set to 3, 2, and 2, respectively).



(d) Circles Dataset (e) k-means (f) AHC

Figure 11: (a)–(i) A plot of the *blobs*, *circles*, and *half-moons* datasets and the clusterings achieved by the *k*-means clustering and agglomerative hierarchical clustering algorithms (where k is set to 3, 2, and 2, respectively).

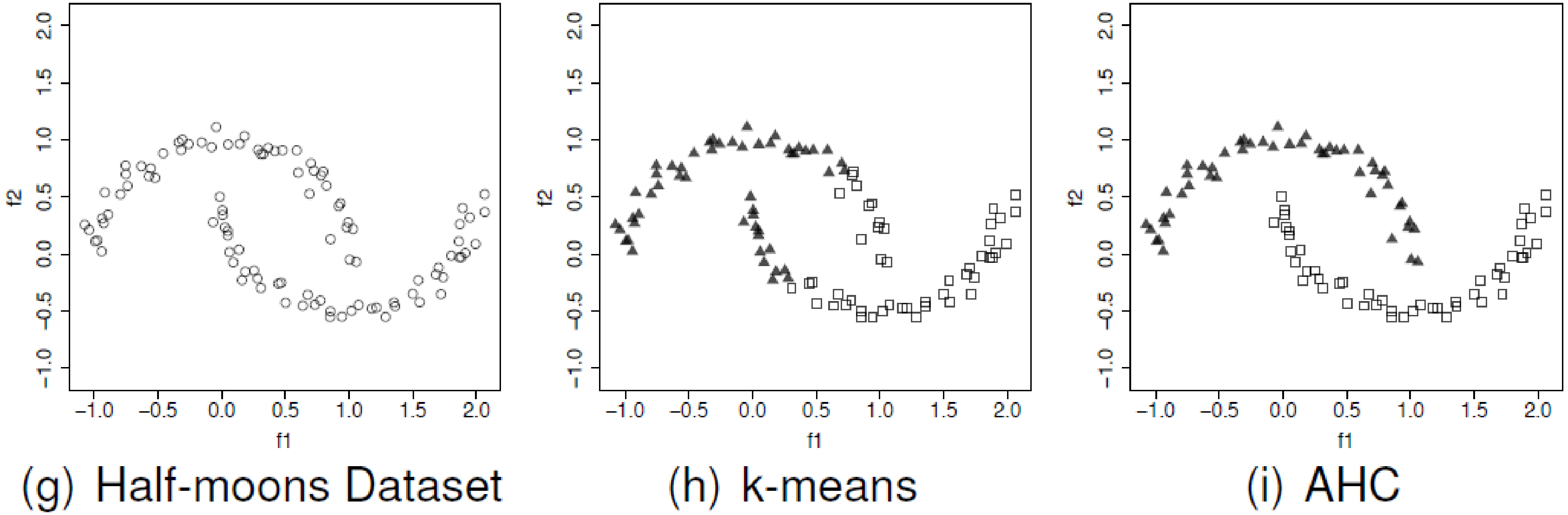


Figure 12: (a)–(i) A plot of the *blobs*, *circles*, and *half-moons* datasets and the clusterings achieved by the k-means clustering and agglomerative hierarchical clustering algorithms (where k is set to 3, 2, and 2, respectively).

Pseudocode description of the **agglomerative hierarchical clustering** algorithm.

Require: a dataset $\mathcal{D}$ containing n training instances, $\mathbf{d}_1, \ldots, \mathbf{d}_n$
Require: a distance measure, $Dist$, to compare distances between instances
Require: a linkage method, $\mathcal{L}$, to compare distances between clusters

```
initialize the hierarchy level, h = 1
divide D into a set of n disjoint clusters, C = {C_1, ..., C_n}, with one instance in each cluster
repeat
    using distance measure Dist and linkage method L, find the nearest pair of clusters, C_i and C_j, in the current clustering
    merge C_i and C_j to form a new cluster C_{n+h}
    remove the old clusters from the clustering: C ← C \ {C_i, C_j}
    add the new cluster to the clustering: C ← C ∪ C_{n+h}
    h ← h + 1
until all the instances join into a single cluster
```

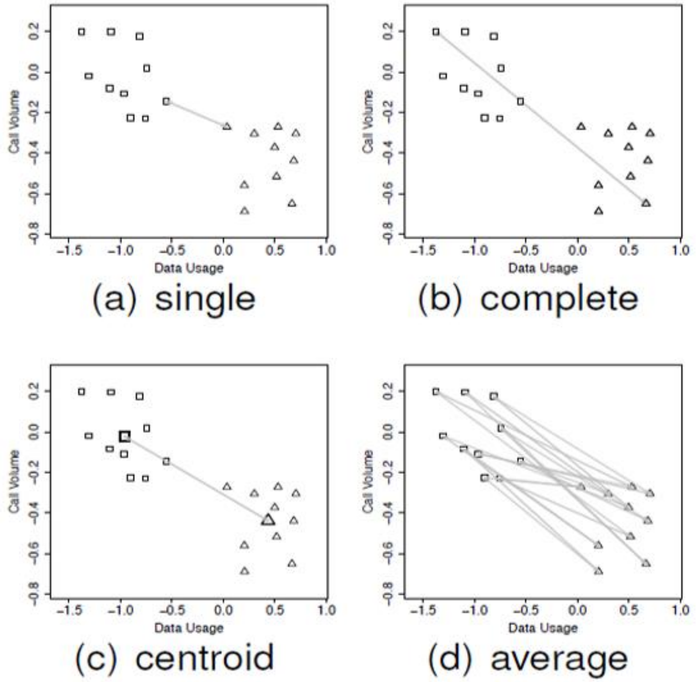


Figure 13: (a)–(d) Different linkage methods that can be used to compare the distances between clusters in agglomerative hierarchical clustering.

Table 5: **Distance matrices** that detail the first three iterations of the AHC algorithm applied to the reduced version of the mobile phone customer dataset in Table 1[10].

(a) A distance matrix for the instances in the dataset.

	d_4	d_{15}	d_8	d_{11}	d_5	d_{19}	d_{24}	d_7	d_{23}
d_4	0.00								
d_{15}	0.28	0.00							
d_8	0.28	0.06	0.00						
d_{11}	2.12	1.89	1.94	0.00					
d_5	2.25	2.02	2.06	0.18	0.00				
d_{19}	2.19	1.95	2.00	0.16	0.07	0.00			
d_{24}	1.66	1.39	1.42	0.81	0.83	0.76	0.00		
d_7	1.84	1.56	1.58	0.96	0.94	0.89	0.27	0.00	
d_{23}	1.79	1.51	1.53	1.08	1.06	1.00	0.33	0.12	0.00

(b) The distance matrix after one iteration of AHC.

	d_4	$\mathcal{C}_{10}$	d_{11}	d_5	d_{19}	d_{24}	d_7	d_{23}
d_4	0.00							
$\mathcal{C}_{10}$	0.28	0.00						
d_{11}	2.12	1.89	0.00					
d_5	2.25	2.02	0.18	0.00				
d_{19}	2.19	1.95	0.16	0.07	0.00			
d_{24}	1.66	1.39	0.81	0.83	0.76	0.00		
d_7	1.84	1.56	0.96	0.94	0.89	0.27	0.00	
d_{23}	1.79	1.51	1.08	1.06	1.00	0.33	0.12	0.00

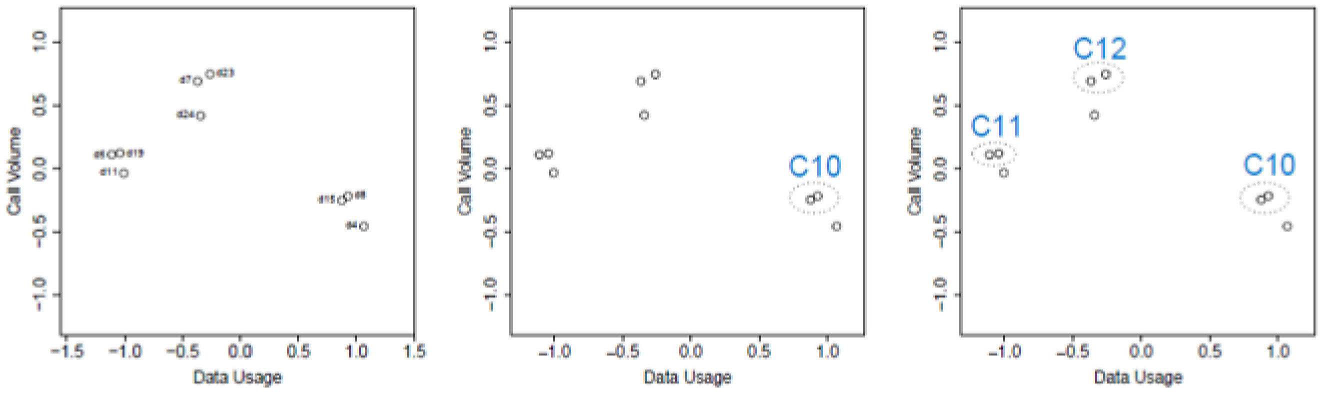
Table 6: **Distance matrices** that detail the first three iterations of the AHC algorithm applied to the reduced version of the mobile phone customer dataset in Table 1[10].

(c) The distance matrix after two iterations of AHC.

	d_4	c_{10}	d_{11}	c_{11}	d_{24}	c_{12}
d_4	0.00					
c_{10}	0.28	0.00				
d_{11}	2.12	1.89	0.00			
c_{11}	2.19	1.95	0.16	0.00		
d_{24}	1.66	1.39	0.81	0.76	0.00	
c_{12}	1.79	1.51	0.97	0.89	0.27	0.00

(d) The distance matrix after three iterations of AHC.

	d_4	c_{13}	c_{11}	d_{24}	c_{12}
d_4	0.00				
c_{13}	0.28	0.00			
c_{11}	2.19	0.16	0.00		
d_{24}	1.66	0.81	0.76	0.00	
c_{12}	1.79	0.97	0.89	0.27	0.00



(a) (b) (c)

Figure 14: (a) A plot of a reduced version of the mobile phone customer dataset given in Table 1[10]. (b) At the first iteration of the AHC algorithm the first pair of instances is combined into a cluster, $\mathcal{C}_{10}$. (c) After three iterations of the AHC algorithm, three pairs of instances have been combined into clusters, $\mathcal{C}_{10}$, $\mathcal{C}_{11}$, and $\mathcal{C}_{12}$. (d) At the fourth iteration of AHC, the first hierarchical cluster combination is created when a single instance, d_{11} is combined with the cluster $\mathcal{C}_{\cancel{10}}$ C11 to create a new cluster, $\mathcal{C}_{13}$.

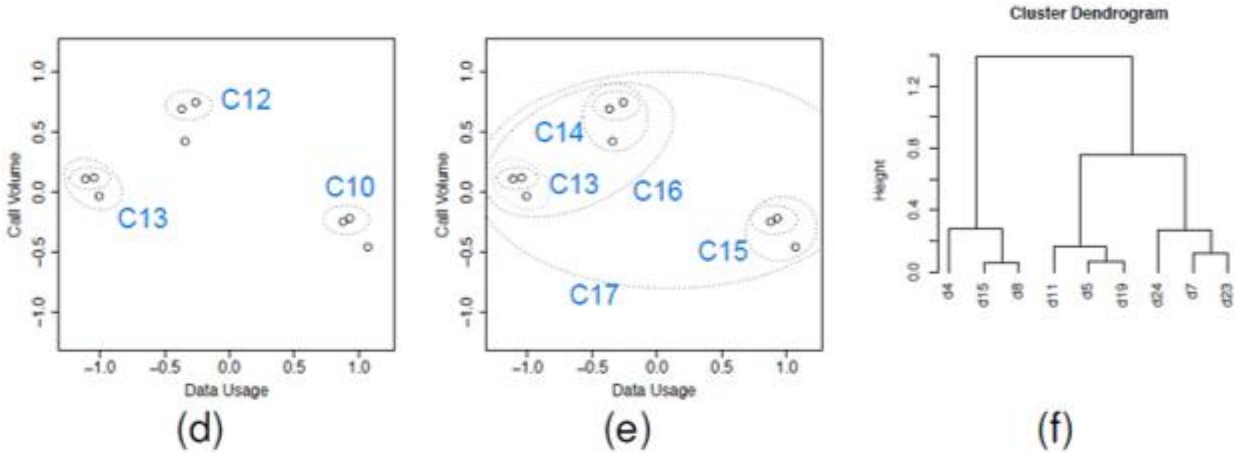
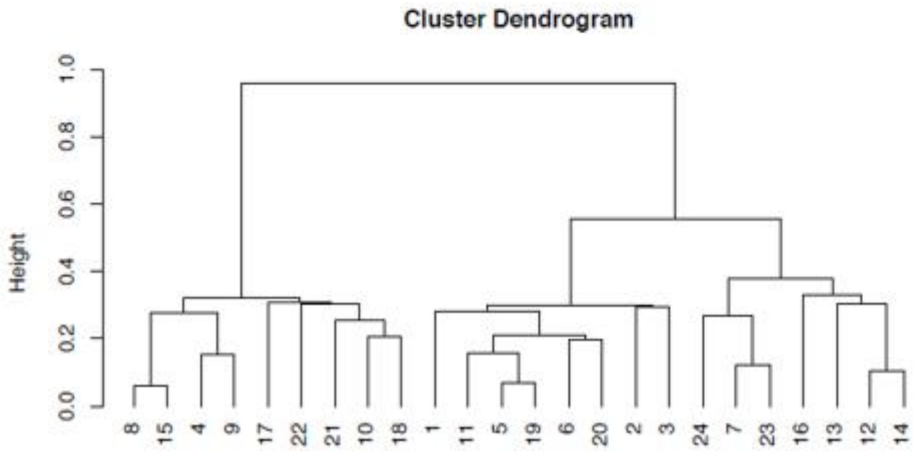
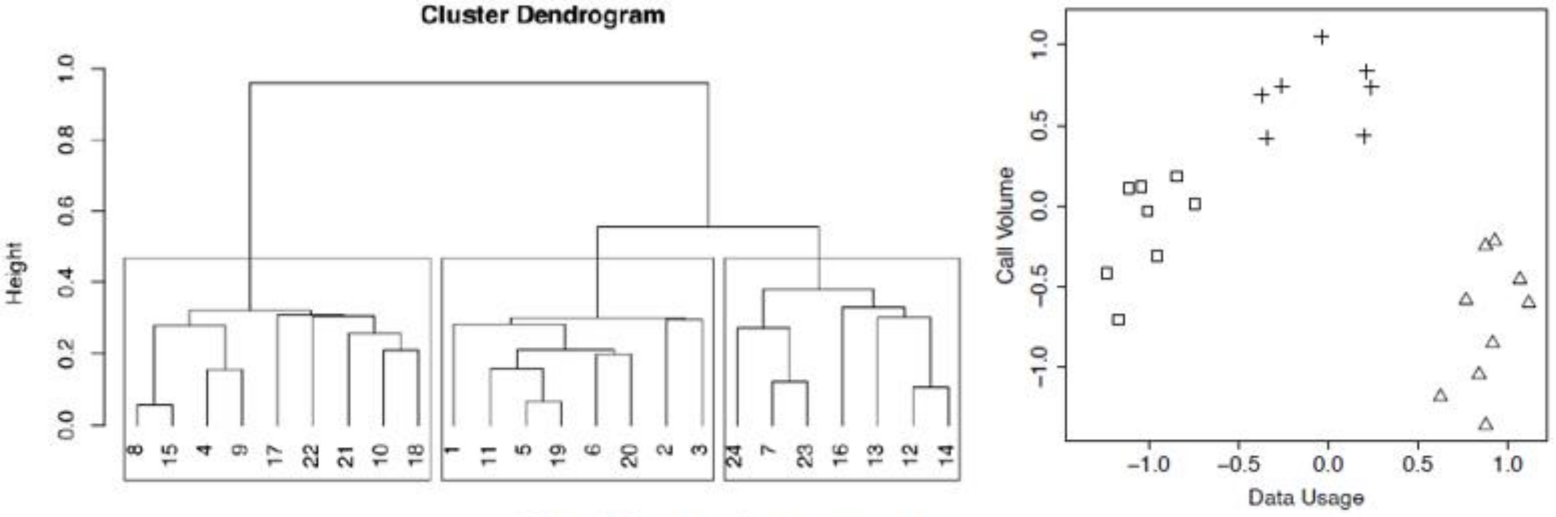


Figure 15: (a) A plot of a reduced version of the mobile phone customer dataset given in Table 1[10]. (b) At the first iteration of the AHC algorithm the first pair of instances is combined into a cluster, $\mathcal{C}_{10}$. (c) After three iterations of the AHC algorithm, three pairs of instances have been combined into clusters, $\mathcal{C}_{10}$, $\mathcal{C}_{11}$, and $\mathcal{C}_{12}$. (d) At the fourth iteration of AHC, the first hierarchical cluster combination is created when a single instance, d_{11} is combined with the cluster $\cancel{\mathcal{C}_{10}}$ C11 to create a new cluster, $\mathcal{C}_{13}$.



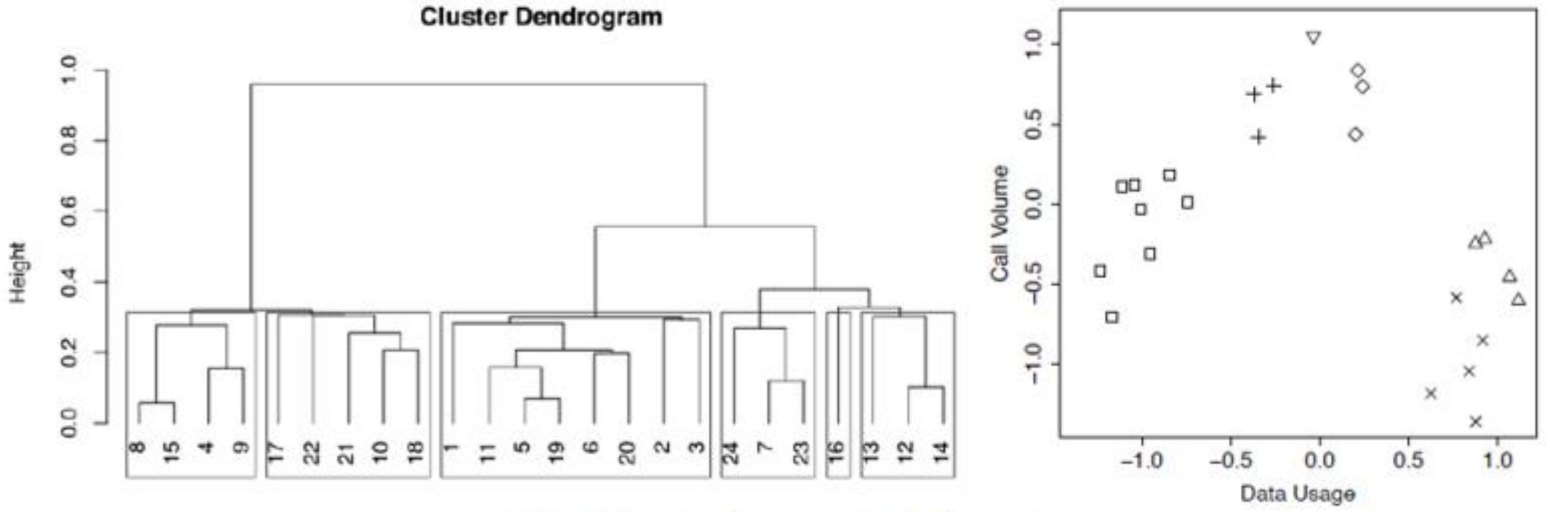
(a) AHC result

Figure 16: (a) A plot of the hierarchical grouping of the instances in the mobile phone customer dataset from Table 1[10] found by the AHC algorithm (using Euclidean distance and single linkage). (b) The clustering returned when the tree is cut at $k = 3$. (c) The clustering returned when the tree is cut at $k = 6$.



(b) Clustering cut at $k = 3$

Figure 17: (a) A plot of the hierarchical grouping of the instances in the mobile phone customer dataset from Table 1[10] found by the AHC algorithm (using Euclidean distance and single linkage). (b) The clustering returned when the tree is cut at $k = 3$. (c) The clustering returned when the tree is cut at $k = 6$.



(c) Clustering cut at $k = 6$

Figure 18: (a) A plot of the hierarchical grouping of the instances in the mobile phone customer dataset from Table 1[10] found by the AHC algorithm (using Euclidean distance and single linkage). (b) The clustering returned when the tree is cut at $k = 3$. (c) The clustering returned when the tree is cut at $k = 6$.

Summary

- Unsupervised machine learning techniques are used in the absence of a target feature and model the underlying structure within the descriptive features in a dataset.
- We can think of the output of most unsupervised machine learning models as new generated features that can be appended to the original dataset to augment or enrich it.
- Two clustering techniques were presented in detail: k-means clustering and agglomerative hierarchical clustering (AHC).
- Applications of unsupervised learning are widespread, including customer segmentations, anomaly detection, and analyzing people’s movement patterns.
- Designing solutions based on unsupervised machine learning techniques can be quite creative.
- Finally, unsupervised learning is a fascinating research area and has many significant open research challenges.