



NUS
National University
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| **Computing**

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Computer Science

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Week 13

CS2109s TG35,36

- 1 K-means algorithm
- 2 Hierarchical clustering
- 3 SVD
- 4 Wrapping up

Student Feedback on Teaching (SFT)

NUS Student Feedback <https://blue.nus.edu.sg/blue/>:

- › Don't Mix module/grading/project feedback - **feedback only for teaching.**
- › Feedback is confidential to university and anonymous to us.
- › Feedback is optional but highly encouraged.
- › Past student feedback improves teaching; see <https://www.eric-han.com/teaching>
 - ›› ie. Telegram access, More interactivity.
- › Your feedback is important to me, and will be used to improve my teaching.
 - ›› Good > Positive feedback > Encouragement
 - Teaching Awards (nominate)
 - Steer my career path
 - ›› Bad > Negative feedback (nicely pls) > Learning
 - Improvement
 - Better learning experience

In case you want to go and review some of our bonus questions, Wenzhong from TG04/2324s1 (some differences) has completed them all! With permission from him, he have agreed to share his solutions with all of you:

<https://github.com/LWZ19/CS2109s-2324s1-bonus>



Section 1: **K-means** algorithm



Algorithm 1: K-means clustering

```
1 for  $k = 1$  to  $K$  do
2    $\mu_k \leftarrow$  random location
3 while not converged do
4   for  $i = 1$  to  $m$  do
5      $c^{(i)} \leftarrow \operatorname{argmin}_k \|x^{(i)} - \mu_k\|^2$ 
6   for  $k = 1$  to  $K$  do
7      $\mu_k \leftarrow \frac{1}{|\{x^{(i)} | c^{(i)} = k\}|} \sum_{x \in \{x^{(i)} | c^{(i)} = k\}} x$ 
```

Recap

- 1 What is the key idea between K-means?

Prove that the algorithm...

- i. always produces a partition with a lower loss (monotonically decreasing)
- ii. always converges ¹.
- iii. [©] What is EM algorithm and does it relate to K-Means?

Fun Fact: K-Means is my first ML algorithm that I implemented.

¹centroids/medoids do not change after an iteration

Answer

- a. Always produces a partition with a lower or eq loss...
 - a. Fix assignment, find the mean points ($|a + b|^2 = |a|^2 + |b|^2 + 2 \langle a, b \rangle$)
 - b. Fix mean point, find the new assignment. (By definition of L5)
- b. Always converges... (pigeonhole principle + loss never increases)
 - a. There are k^N possible config to partition N data points into k clusters
 - b. So we are transiting from one config to the next.
 - c. The next config has lower or eq loss
 - d. There cannot be a cycle where the next is always lower.
 - e. So must converge in finite number of iterations.

Question 2

Although k-means always converges, it may get stuck at a bad local minimum. What are some ways to help?

Recap

- 1 Run the algorithm multiple times, what happens?

Answer

The issue is with the initialization:

- 1 Choose the first centroid randomly then the next to be as far as possible from the first, etc...
- 2 K-means++, first centroid randomly and choose the rest using some probability distribution.

Question 3

i	1	2	3	4	5	6
x	1	1	2	2	3	3
y	0	1	1	2	1	2

Table 1: 6 data points on a 2D-plane

Cluster the 6 points in table 1 into **two** clusters using the K-means algorithm. The two initial centroids are $(0, 1)$ and $(2.5, 2)$.

Answer

Iteration 1

Using first centroid = (0, 1) and second centroid = (2.5, 2), we get the table below.

Point	D^2 to first centroid	D^2 to second centroid	Assigned Cluster
1	2	6.25	1
2	1	3.25	1
3	4	1.25	2
4	5	0.25	2
5	9	1.25	2
6	10	0.25	2

Computing the new centroids:

- › Centroid 1 = $((1, 0) + (1, 1)) / 2 = (1, 0.5)$
- › Centroid 2 = $((2, 1) + (2, 2) + (3, 1) + (3, 2)) / 4 = (2.5, 1.5)$

Iteration 2

Using first centroid = (1, 0.5) and second centroid = (2.5, 1.5), we get the table below.

Point	D^2 to first centroid	D^2 to second centroid	Assigned Cluster
1	0.25	4.5	1
2	0.25	2.5	1
3	1.25	0.5	2
4	3.25	0.5	2
5	4.25	0.5	2
6	6.25	0.5	2

Computing the new centroids:

- › Centroid 1 = $((1, 0) + (1, 1)) / 2 = (1, 0.5)$
- › Centroid 2 = $((2, 1) + (2, 2) + (3, 1) + (3, 2)) / 4 = (2.5, 1.5)$

Since the centroids are the same as those from the previous iteration, the K-means algorithm has converged.

Question 4

Cluster the 6 points in table 1 into **two** clusters using the K-medoids algorithm. The initial medoids are point 1 and point 3.

Recap

- 1 What is the key difference between K-means and K-medoids?

Answer

Iteration 1

Point	D^2 to first medoid	D^2 to second medoid	Assigned Cluster
1	0	2	1
2	1	1	2
3	2	0	2
4	5	1	2
5	5	1	2
6	8	2	2

For point 2, the distance between itself to the first medoid is the same as the distance between itself to the second medoid.

- For simplicity, we assign point 2 as a member of the second cluster.
- The strategy chosen must be deterministic.

Computing the new medoid:

- › Centroid 1 = (1, 0)
- › Centroid 2 = $((1, 1) + (2, 1) + (2, 2) + (3, 1) + (3, 2)) / 5 = (2.2, 1.4)$

We need to find the closest points to each centroid.

- › For centroid 1, the closest point is point 1. Hence, we set point 1 as the new medoid.
- › For centroid 2, the closest point is point 3. Hence, we set point 3 as the new medoid.

Since the medoids are the same as the initial ones, the K-medoids algorithm has converged.



Section 2: **Hierarchical clustering**



Given this dataset:

i	1	2	3	4	5
x_1	0	1	3	1	1
x_2	0	1	0	3	4

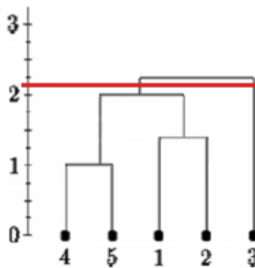
- 1 Complete the distance matrix (using square of Euclidean distance).
- 2 Draw the dendrogram for the three linkage methods (Single, Complete and Centroid).
- 3 Draw a line that partitions it into 2 clusters.

Recap

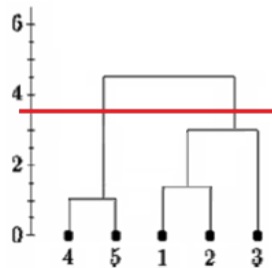
What is the algorithm to construct a hierarchical cluster?

Answer

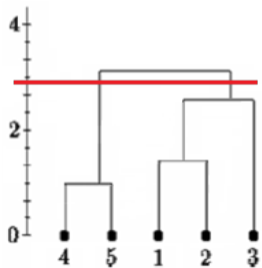
	1	2	3	4	5
1	0				
2	2	0			
3	9	5	0		
4	10	4	13	0	
5	17	9	20	1	0




(a) Single linkage



(b) Complete linkage



(c) Centroid linkage



Section 3: **SVD**

Using the `tut10.ipynb`, we study PCA:

- 1 The current choice of $k = 9$ does not produce a very nice output. What is a good value for k ?
- 2 For the value of k you select in (a), what is the space saved by doing this compression?
- 3 What are the drawbacks of this form of compression?
- 4 [©] How does JPEG work and relate to this technique?
- 5 [©] Should we mean-center the data? How does the calculation change?
- 6 [©] What happens when we use the largest k ?

Recap

- › What is PCA and how does it work?

Answer 1



Figure 2: $k = 286$ gives us 99% of the variance

Answer 2

When using $k = 286$, the (512×1536) 2D-array is now represented by U_{reduce} (512×286) and Z (286×1536). This demonstrates approximately 25.5% space saved.

$$\frac{(512 \times 286) + (286 \times 1536)}{512 \times 1536} = \frac{585728}{786432} = 0.745$$

If we wish to have more compression, we can choose a smaller k , but at the expense of image quality.

Answer 3

- › Lossy Compression - The image cannot be reconstructed exactly and permanently loses information - ie. 100% of variance.
- › Using the full U_{reduce} , we actually use more space than the original.



Section 4: **Wrapping up**



- › NUS: 2023 GES Employment Rates
- › AI Hype comes in cycles.
- › Do what interest you - I picked AI/ML because I love it.

Recommended Next Modules (If you like AI?)

- › CS3263 - Foundations of Artificial Intelligence
- › CS3264 - Foundations of Machine Learning
- › CS5339 - Theory and Algorithms for Machine Learning
- › CS5340 - Uncertainty Modelling in AI
- › CS5446 - AI Planning and Decision Making
- › CS5242 - Neural Networks and Deep Learning
- › Project Modules (FYP/CP4106)
 - ›› AI driven Modern Web Crawling
 - ›› Numerical accuracy in Bayesian Optimization
 - ›› Visualising Machine Learning Algorithms
 - ›› (Or propose your own)

- 1 [©] and Bonus declaration is to be done here; You should show bonus to Eric.
- 2 Attempted tutorial should come with proof (sketches, workings etc...)
- 3 Random checks may be conducted.
- 4 Guest student should come and inform me.



Figure 3: Buddy Attendance: <https://forms.gle/q5Secb3dHshmXNXd7>

