— K-MEANS CLUSTERING

1. THE PROBLEM
2. ILLUSTRATION ON A 1-D EXAMPLE
✓ 3. THE 1-D ALGORITHM
✓ 4. DISTORTION AND ITS MINIMIZATION BY K-MEANS
✓ 5. THE K-MEANS ALGORITHM FOR HIGHER-D DATA
✓ 6. "FAILURE" OF K-MEANS
✓ 7. EXAMPLES AND APPLICATIONS

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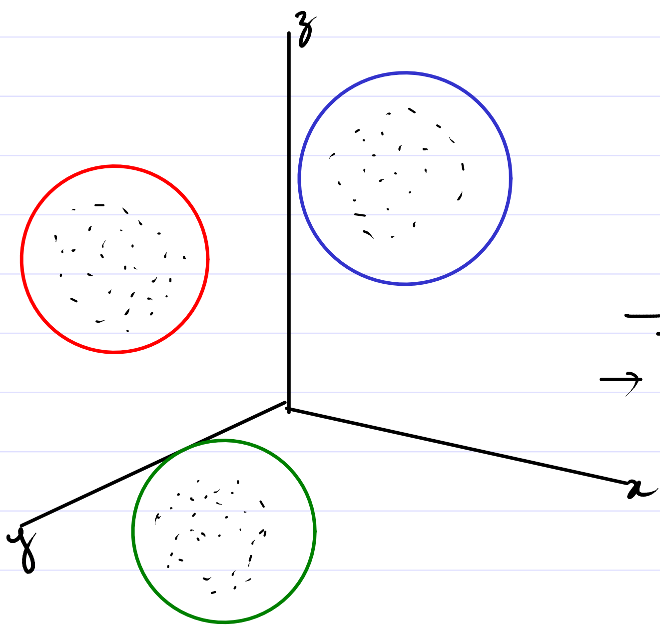
1. PROBLEM



— DATA MATRIX A
— GIVEN k : DESIRED # OF CLUSTERS
— GOAL : FIND BEST k CLUSTERS

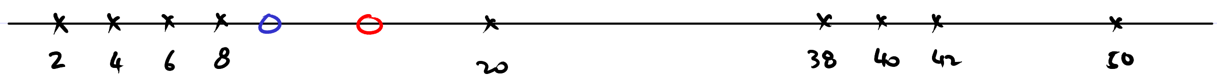
— APPLICATIONS
→ Eg: (SUDS): MOVIE RANKING DATA CLUSTERING

— VERY DIFFICULT : NP-HARD

— K-MEANS CLUSTERING
— GOOD SOLUTIONS QUICKLY : USUALLY
— BUT NO GUARANTEE

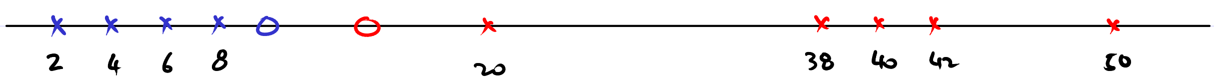
2. 1-D EXAMPLE

→ STEP 0: PICK k=2 CLUSTER CENTERS ("MEANS")



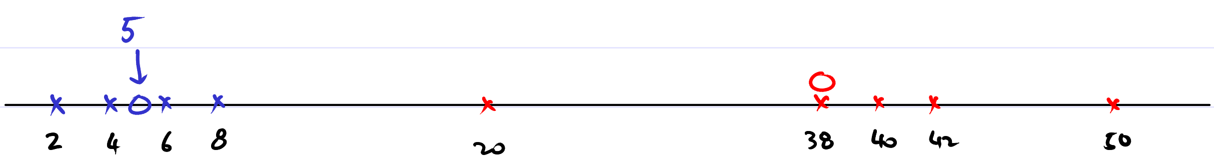
— ROUND 1

— STEP 1: ASSIGN DATA TO NEAREST CLUSTER MEAN



— STEP 2: UPDATE MEANS TO AVG OF CLUSTER DATA

→ CENTROID



$\frac{20}{4} = 5$

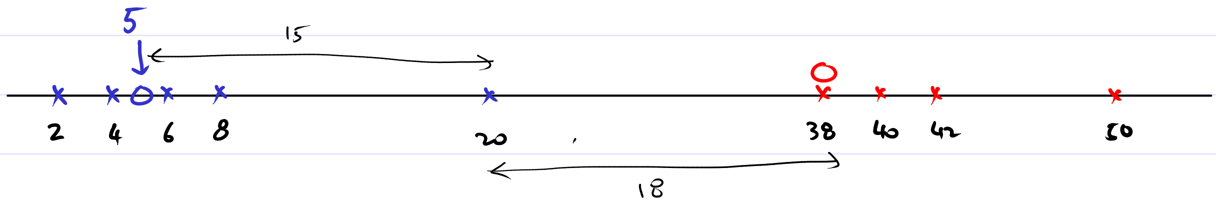
$\frac{20+120+50}{5} = \frac{190}{5} = 38$

— STEP 3: ANY CHANGE → GO TO STEP 1 (NEXT ROUND) ✓

— ELSE: DONE (STOP)

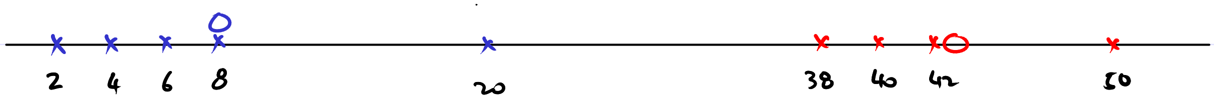
ROUND 2

— STEP 1 : ASSIGN DATA TO NEAREST CLUSTER MEAN



— STEP 2 : UPDATE MEANS TO AVG OF CLUSTER DATA

→ CENTROID

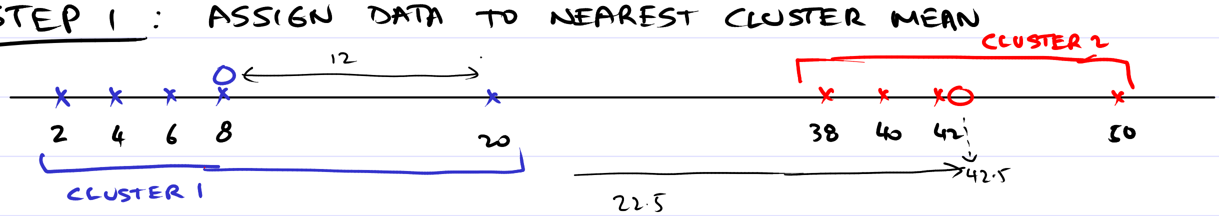


$\frac{20+20}{5} = 8$ $\frac{170}{4} = 42.5$

— STEP 3 : CHANGES? YES → ROUND 3

— ROUND 3

— STEP 1 : ASSIGN DATA TO NEAREST CLUSTER MEAN



— NO CHANGES TO CLUSTER ASSIGNMENT

— STEP 2 : NO CHANGES

— STEP 3 : DONE

3 : 1-D ALGORITHM

$S_1 \quad \ldots \quad S_k \leftarrow$ CLUSTER NAMES

A : CHOOSE k MEANS (CLUSTER CENTERS) : $m_1, \ldots, m_k$

ROUND :

B : ASSIGN DATA TO NEAREST CLUSTER :

$$\underbrace{x_i \longmapsto S_j}_{\text{ASSIGNED TO}}, \quad \text{s.t.} \quad |x_i - \underbrace{m_j}_{\text{mean for } S_j}| \leq |x_i - m_\ell|, \text{ for } \ell = 1, \ldots, k.$$

C : RE-ASSIGN MEANS.

$$\rightarrow \quad m_i \triangleq \frac{1}{|S_i|} \sum_{j=1}^{|S_i|} x_{ij}$$

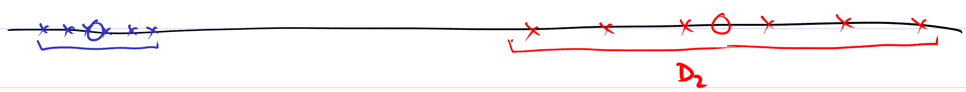
$|S_i| \leftarrow$ the number of data points in S_i

$x_{ij} \leftarrow$ the j^{th} data point in S_i

D. If any changes from prev. round : START NEW ROUND

$\rightarrow$ ELSE : STOP. CLUSTERS FOUND.

4 DISTORTION AND ITS MINIMIZATION



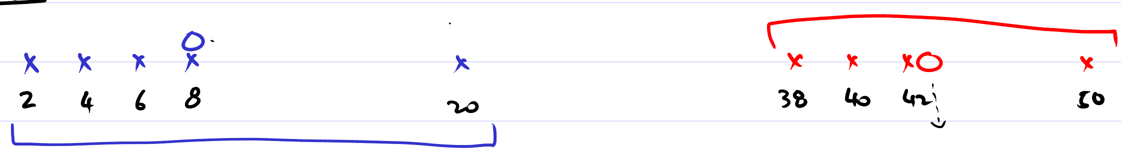
$D_2 > D_1$

→ DISTORTION OF A CLUSTER i (S_i)

$$\rightarrow D_i \triangleq \sum_{j=1}^{|S_i|} (x_{ij} - m_i)^2$$

$$\rightarrow \text{TOTAL DISTORTION: } D = \sum_{i=1}^{k} D_i$$

→ EXAMPLE:



$$D_1 = (2-8)^2 + (4-8)^2 + (6-8)^2 + (8-8)^2 + (20-8)^2 = 200$$

$$D_2 = (38-42.5)^2 + (40-42.5)^2 + (42-42.5)^2 + (50-42.5)^2 = 83$$

$$D = D_1 + D_2 = 283$$

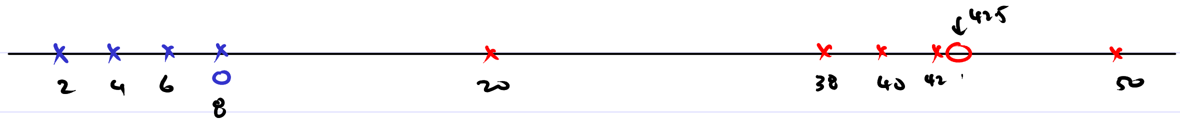
$$\rightarrow \text{Variance of } S_i = \frac{D_i}{|S_i|}$$

→ K-MEANS and DISTORTION

→ STEPS 1 & 2 OF K-MEANS EACH MINIMIZE DISTORTION

→ STEP 1: (MEANS FIXED) DATA ASSIGNED TO NEAREST MEAN

→ CHANGE DATA POINT ASSIGNMENT → INCREASE D



→ $D = 283$; CONTRIBUTION OF 20: $(20-8)^2 = 12^2 = 144$

→ Re-assign 20 → RED

→ CONTRIB OF 20: $(20 - 42.5)^2 = 22.5^2 = 506.25 > 144$

→ K-MEANS' STEP 1 MINIMIZES TOTAL DISTORTION ← w MEANS FIXED

→ STEP 2: MEANS SET TO CLUSTER AVGS (CLUSTER ASSIGNMENTS FIXED)

→ THE CHOICE OF MEAN FOR EACH S_i MINIMIZES D_i

→ Proof:

→ $$D_i = \sum_{j=1}^{|S_i|} (x_{ij} - m_i)^2$$

↳ change this to $p \neq$ avg. of data necessarily

→ $$\hat{D}_i = \sum_{j=1}^{|S_i|} (x_{ij} - p)^2$$

→ FIND THE MINIMUM OF $\hat{D}_i$ as p changes

→ $$\frac{\partial \hat{D}_i}{\partial p} = \sum_{j=1}^{|S_i|} -2(x_{ij} - p) = 0$$ for a minimum

→ $$\sum_{j=1}^{|S_i|} x_{ij} - \underbrace{\sum_{j=1}^{|S_i|} p}_{|S_i| p} = 0$$

→ $$p = \frac{1}{|S_i|} \sum_{i=1}^{|S_i|} x_{ij}$$ ← avg of the data, i.e, m_i

→ (IF THE CLUSTERS ARE FIXED)

→ STEP 2 MINIMIZES D_i for each cluster

HENCE MINIMIZES $\sum D_i = D$

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5. K-MEANS FOR GENERAL HIGHER DIMENSIONAL DATA

A: CHOOSE k MEANS (CLUSTER CENTERS): $\overset{S_1}{\vec{m}_1}, \ldots, \overset{S_k}{\vec{m}_k}$ ← CLUSTER NAMES

ROUND:

(STEP 1) B: ASSIGN DATA TO NEAREST CLUSTER:

$$\vec{x}_i \underset{\text{ASSIGNED TO}}{\longmapsto} S_j, \quad \text{s.t.} \quad \|\vec{x}_i - \underbrace{\vec{m}_j}_{\text{mean for } S_j}\| \le \|\vec{x}_i - \vec{m}_\ell\|, \text{ for } \ell = 1, \ldots, k.$$

(STEP 2) C: RE-ASSIGN MEANS.

$|S_i|$ ← the number of data points in S_i

$$\rightarrow \vec{m}_i \triangleq \frac{1}{|S_i|} \sum_{j=1}^{|S_i|} \vec{x}_{ij}$$ ← the j^{th} data point in S_i

D. If any changes from prev. round: START NEW ROUND

→ ELSE: STOP. CLUSTERS FOUND.

→ DISTORTION OF A CLUSTER i (S_i)

$$\rightarrow D_i \triangleq \sum_{j=1}^{|S_i|} \|\vec{x}_{ij} - \vec{m}_i\|^2$$

$$\rightarrow \text{TOTAL DISTORTION: } D = \sum_{i=1}^{k} D_i$$

→ **MINIMIZATION**

— STEP 1 MINIMIZED D w.r.t CLUSTER ASSIGNMENTS (MEANS CONST)

— STEP 2 " " " CHOICE OF MEANS (CLUSTERS CONST)

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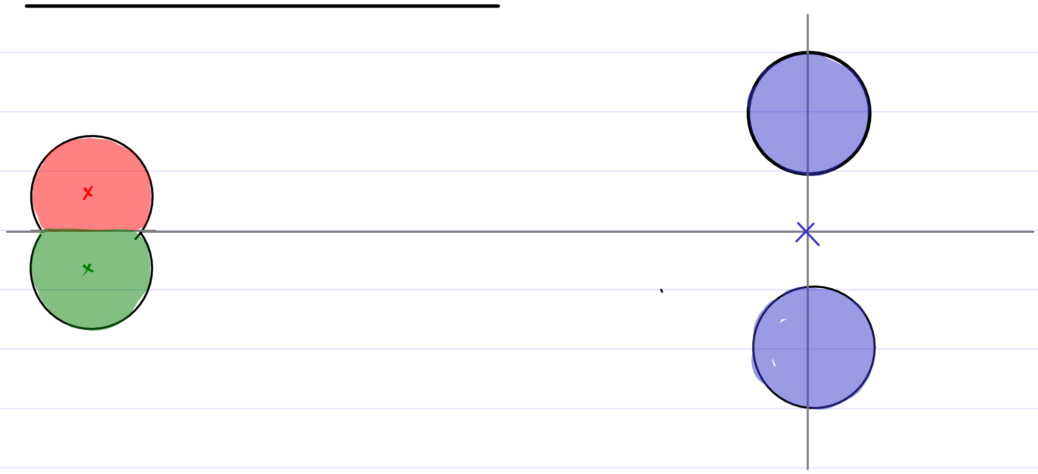
6. "FAILURE" OF K-MEANS



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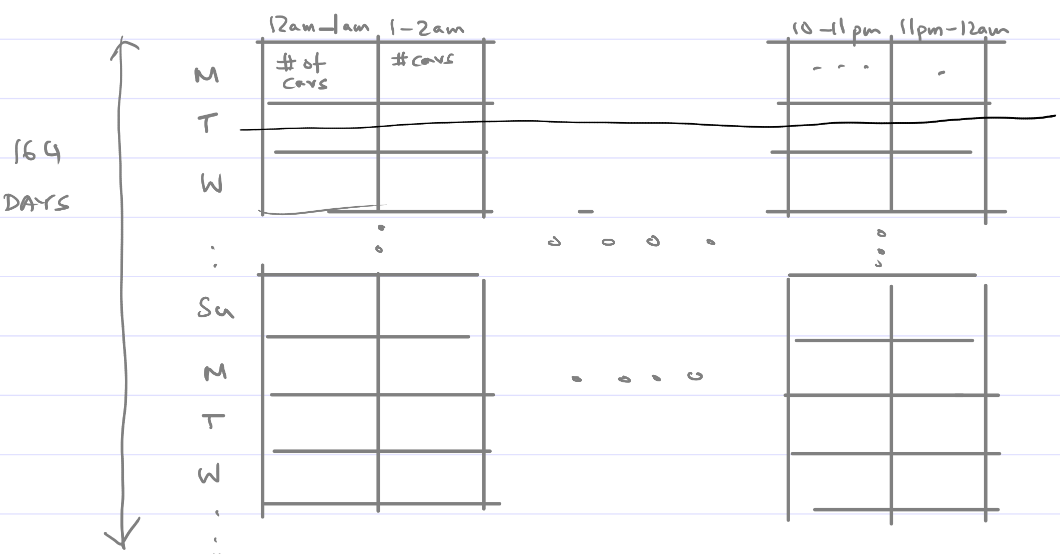
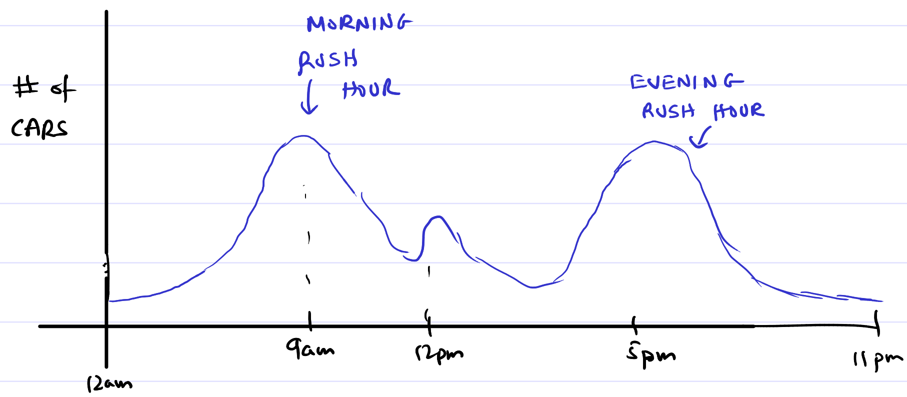
7. TRAFFIC PATTERN ANALYSIS





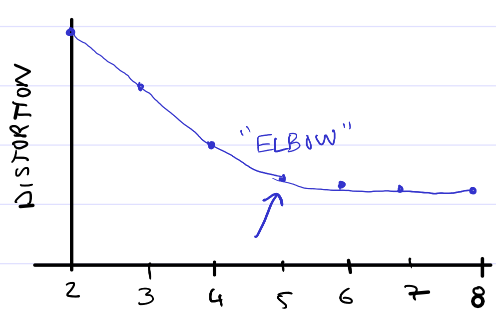
⟶ CLUSTERED THE DATA FOR 164 DAYS

⟶ INTERSECTION IN S. CAROLINA

⟶ WITH $k=4$, <u>M–Th</u>, <u>F</u>, <u>Sa</u>, <u>Su</u>

— <u>HOW TO CHOOSE k</u> ?

⟶ <u>ELBOW CURVE METHOD</u>



⟶ <u>SUMMARY</u>

— K-MEANS: PUTS DATA INTO k CLUSTERS

— MOSTLY WORKS WELL, NO GUARANTEE.

— METRIC: DISTORTION ⟶ HOW GOOD THE CLUSTERING

⟶ K-MEANS REDUCES DISTORTION IN EACH STEP

— IMPORTANT DATA ANALYSIS TECHNIQUE

⟶ COMPLEMENTS PCA / SVD.