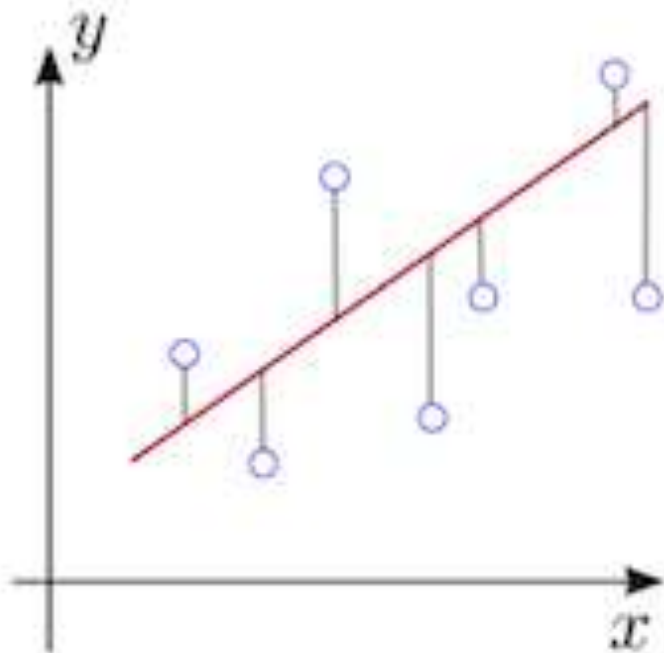
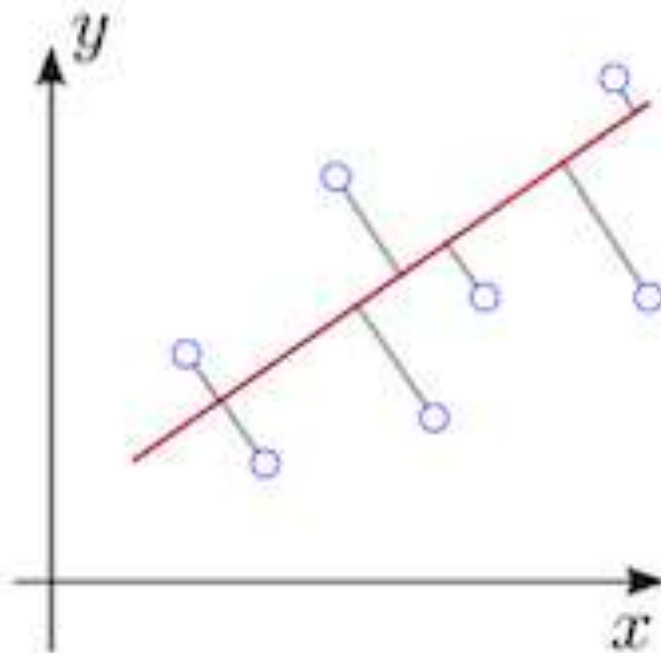


# OLS and TLS

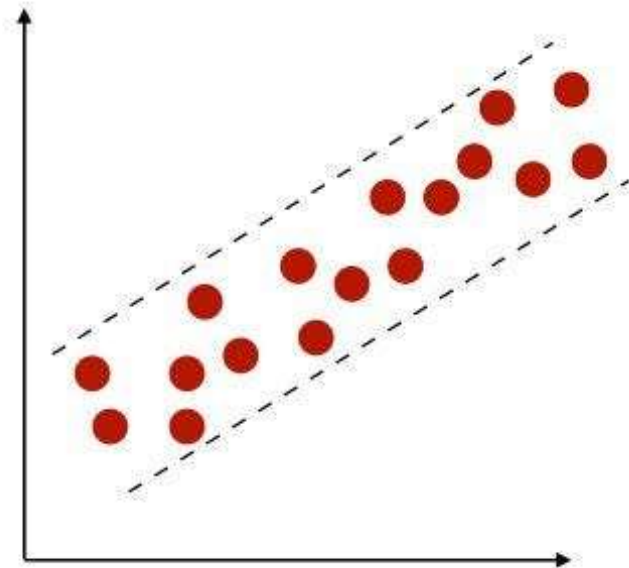
OLS



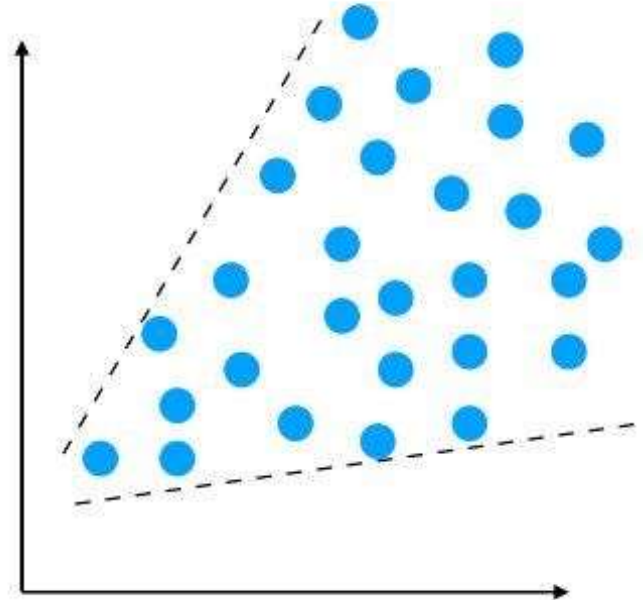
TLS



# Homo/Heteroscedasticity



Homoscedasticity



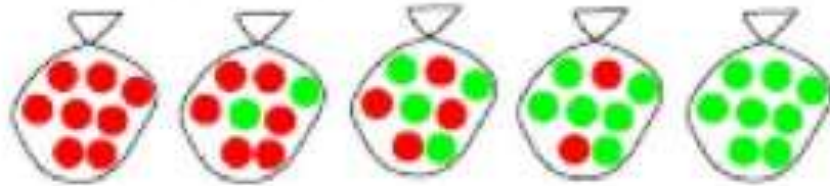
Heteroscedasticity

$$\text{PROBABILITY} = \frac{\text{EVENT}}{\text{OUTCOMES}}$$



# Data – a probability-based perspective

- The basis for Statistical Learning Theory



Then we observe candies drawn from some bag: ●●●●●●●●●●

- Domain described by random variables (r.v.)
  - $X = \{\text{apple, grape}\}$
  - $b_i \in [1,5]$
- **Data = Instantiation of some or all r.v.'s in the domain**

## Uncertainty arises from many sources

### Process Uncertainty

Processes contain  
"randomness"



Uncertain travel times



Semiconductor yield

### Data Uncertainty

Data input is uncertain



GPS Uncertainty



Testimony



{Paris Airport}

Ambiguity



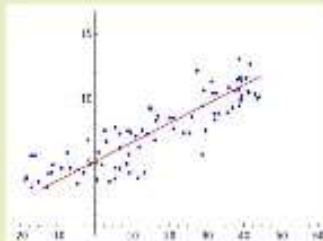
Contaminated?  
Rumors

{John Smith, Dallas}  
{John Smith, Kansas}

Conflicting Data

### Model Uncertainty

All modeling is approximate



Fitting a curve to data



Forecasting a hurricane  
([www.noaa.gov](http://www.noaa.gov))

# Data: a probabilistic perspective

## Output

	DBAName	AKAName	Address	City	State	Zip
t1	John Veliotis Sr.	Johnnyo's	3465 S Morgan ST	Chicago	IL	60608
t2	John Veliotis Sr.	Johnnyo's	3465 S Morgan ST	Chicago	IL	60609
t3	John Veliotis Sr.	Johnnyo's	3465 S Morgan ST	Chicago	IL	60609
t4	Johnnyo's	Johnnyo's	3465 S Morgan ST	Cicago	IL	60608

Conflicts

Does not obey data distribution

Conflict



### Proposed Cleaned Dataset

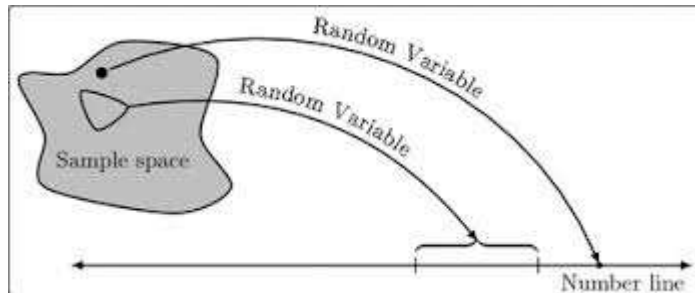
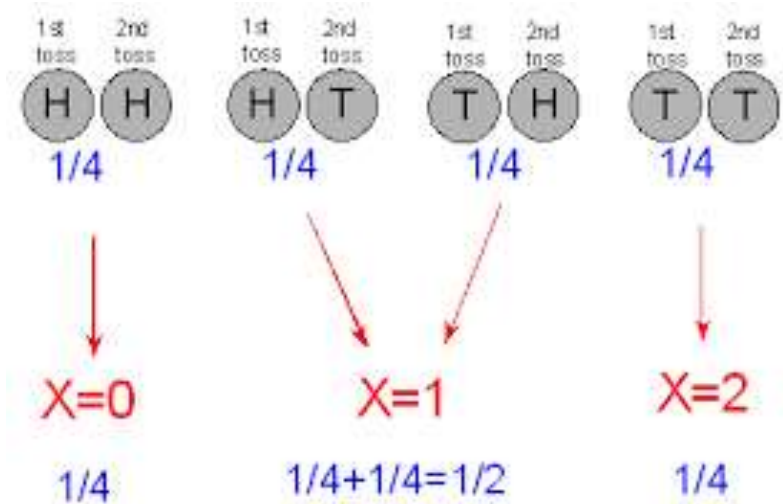
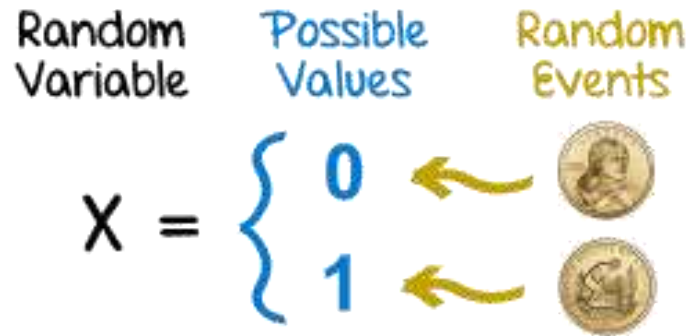
	DBAName	Address	City	State	Zip
t1	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	60608
t2	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	60608
t3	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	60608
t4	John Veliotis Sr.	3465 S Morgan ST	Chicago	IL	60608

### Marginal Distribution of Cell Assignments

Cell	Possible Values	Probability
t2.Zip	60608	0.84
	60609	0.16
t4.City	Chicago	0.95
	Cicago	0.05
t4.DBAName	John Veliotis Sr.	0.99
	Johnnyo's	0.01

# Random Variables

R.V. = A numerical value from a random experiment



# Random variables

- A **discrete random variable** can assume a countable number of values.
  - Number of steps to the top of the Eiffel Tower\*





# Random variables

- A **discrete random variable** can assume a countable number of values.
  - Number of steps to the top of the Eiffel Tower\*
- A **continuous random variable** can assume any value along a given interval of a number line.
  - The time a tourist stays at the top once s/he gets there



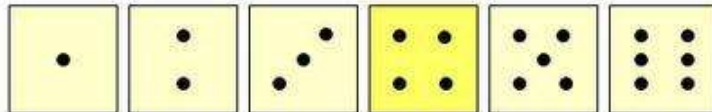
\*Believe it or not, the answer ranges from 1,652 to 1,789. See [Great Buildings](#)



# Discrete Random Variables

- Can only take on a countable number of values

Examples:



- Roll a die twice**

**Let  $X$  be the number of times 4 comes up**  
**(then  $X$  could be 0, 1, or 2 times)**

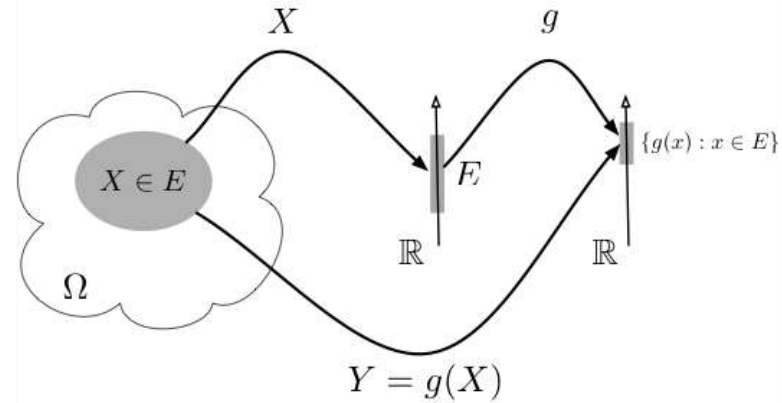
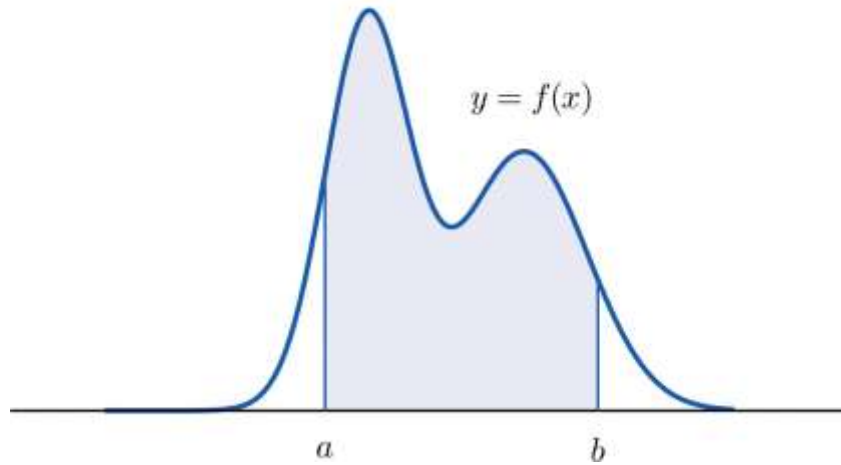
- Toss a coin 5 times.**

**Let  $X$  be the number of heads**  
**(then  $X = 0, 1, 2, 3, 4, \text{ or } 5$ )**

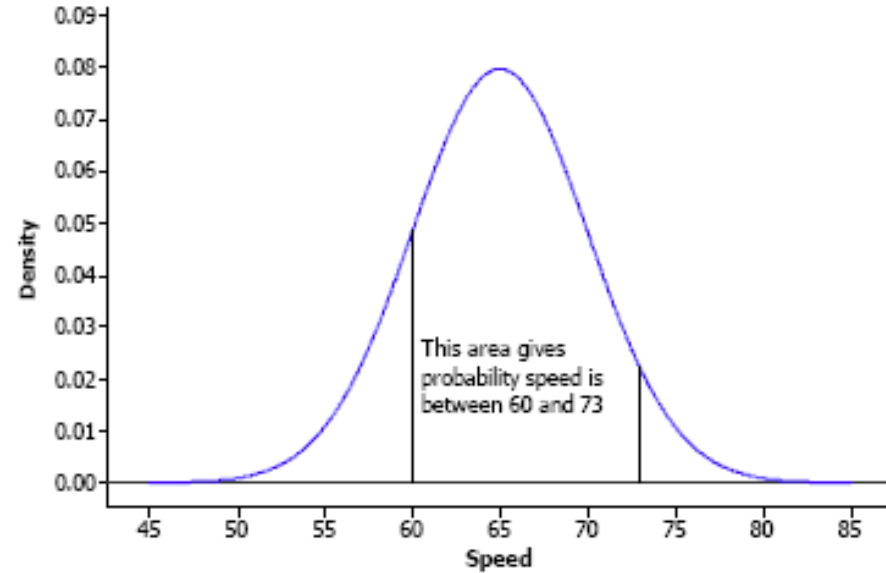
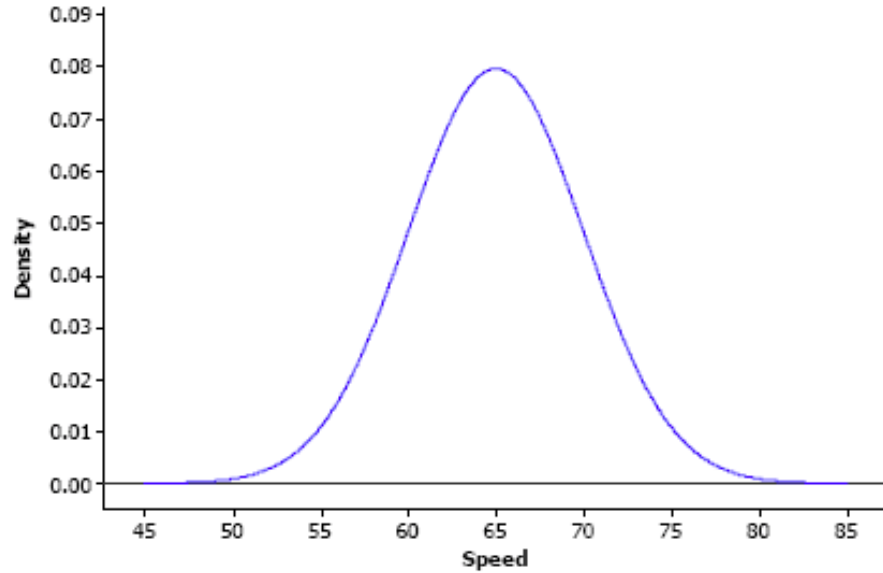


# Continuous random variable

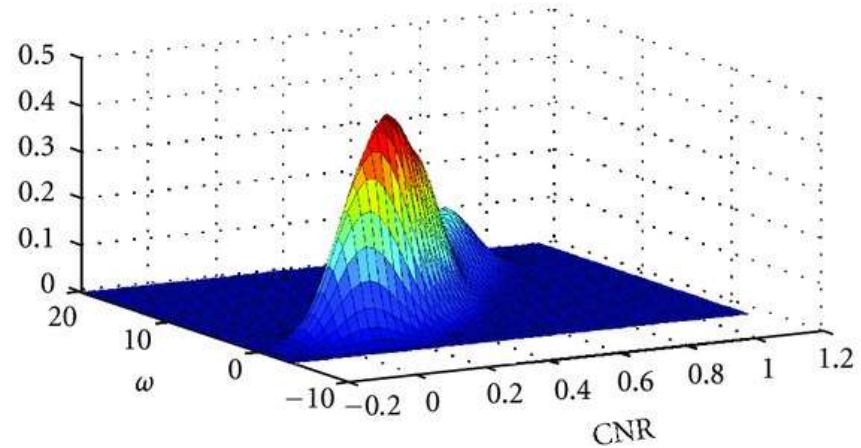
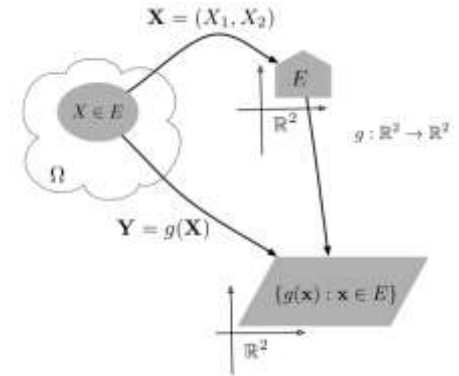
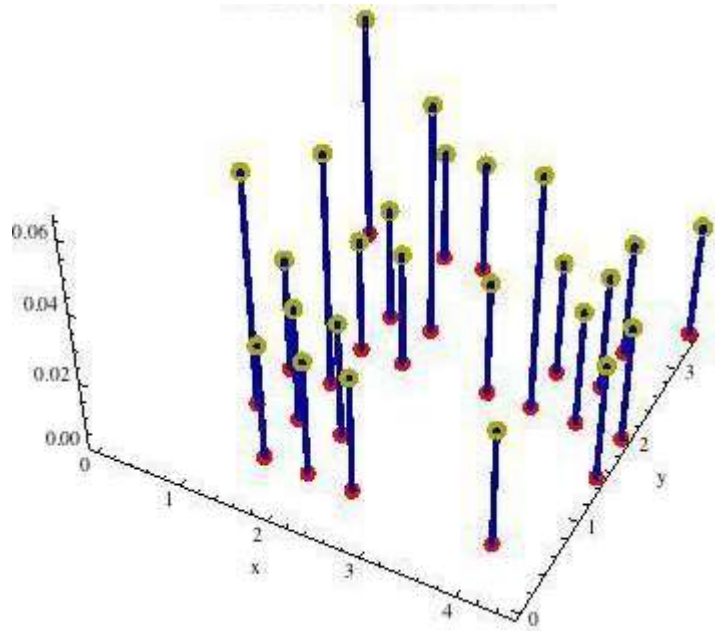
$P(a < X < b) = \text{area of shaded region}$



# Continuous random variable



# Random vectors



# Data $\rightarrow$ r.v.

## Relative frequency

Relative frequency is the same as experimental probability.  
We use relative frequency to predict probabilities from experimental data.

### The experiment

This spinner was spun 40 times and the results recorded in this table:



Colour	Frequency
Blue	20
Yellow	10
Red	5
Green	5

### Relative frequency

$$\frac{\text{frequency of event}}{\text{total number of trials}}$$

**Event** means **one possible outcome**;  
here, one colour on the spinner.

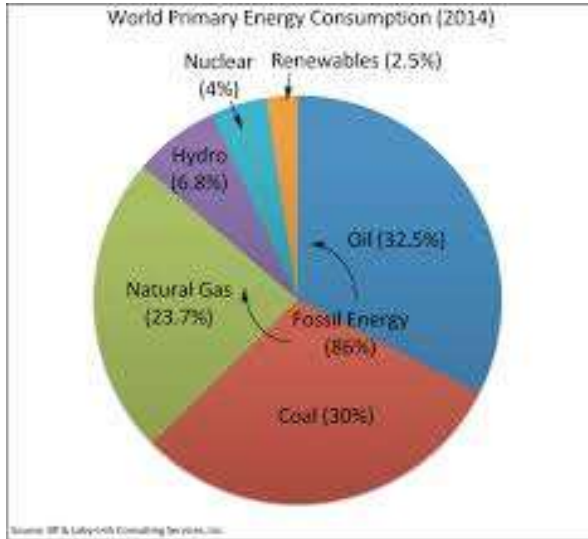
There were 20 blues recorded...

$$P(\text{blue}) = \frac{20}{40}$$

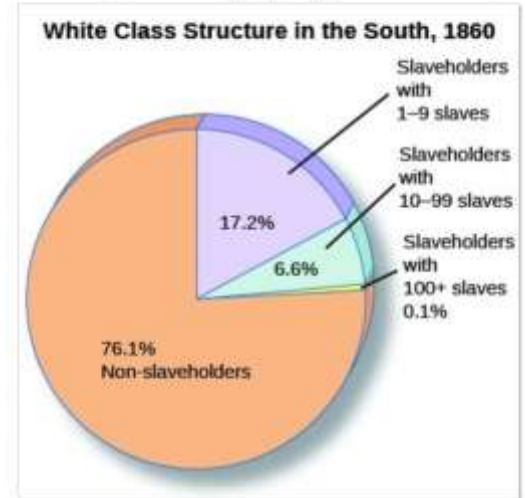
...out of 40 spins.

$$\text{Simplify: } P(\text{blue}) = \frac{20}{40} = \frac{2}{4} = \frac{1}{2}$$

# Discrete Prior distributions

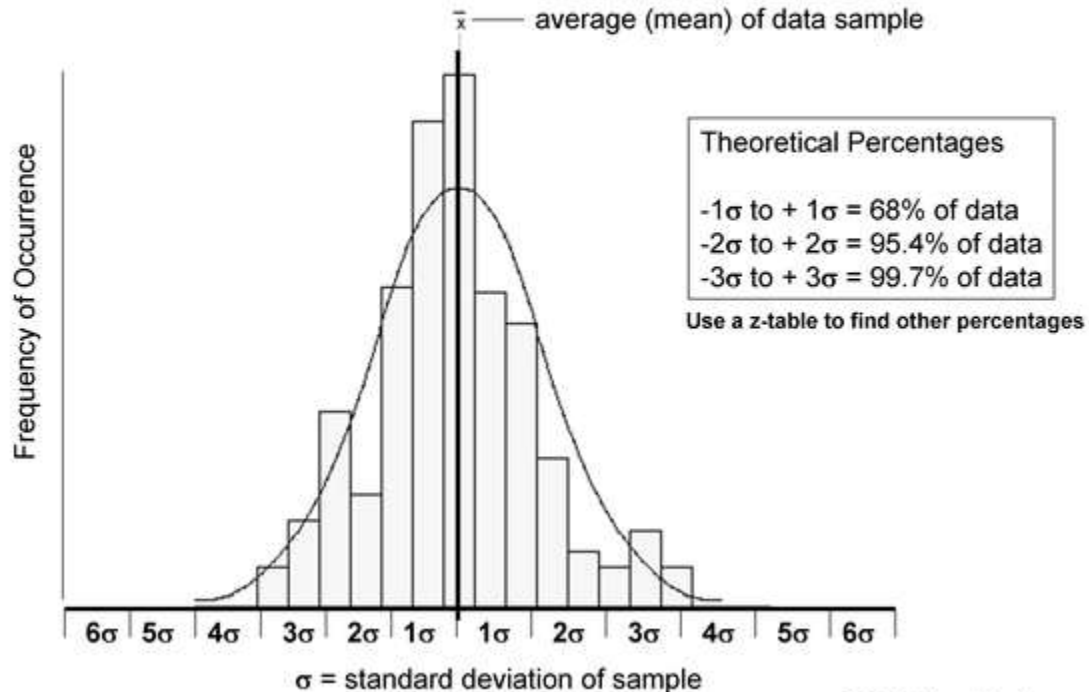


## Slave-Owning Population (1860)



# Data $\rightarrow$ r.v.

Normal Distribution Curve, Fit to a Histogram

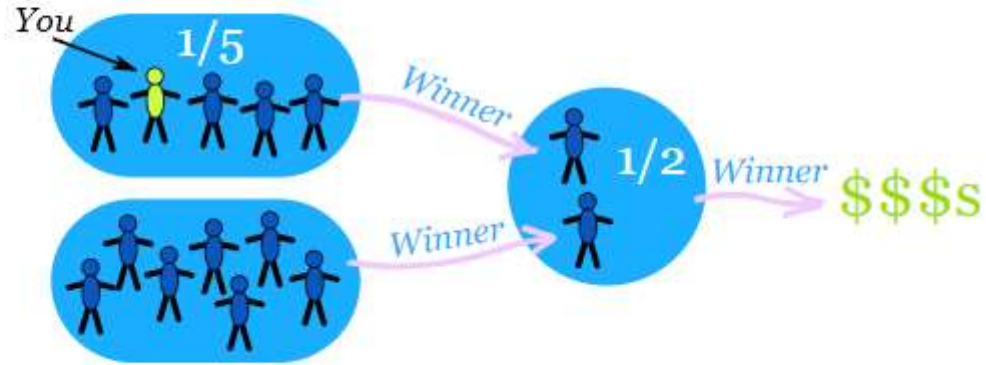




# Independent Events

Imagine there are two groups:

- A member of each group gets randomly chosen for the winners circle,
- **then** one of those gets randomly chosen to get the big money prize:



What is your chance of winning the big prize?

# Independent vs. Dependent Events



Using the bag of marbles on the left, what is the probability of pulling a black marble two times in a row?  $P(\text{black}, \text{black})$

When you put 1<sup>st</sup> marble back in  
(*Independent Events*)

$$\frac{2}{10} * \frac{2}{10}$$

$$\frac{1}{5} * \frac{1}{5} = \frac{1}{25}$$

When you KEEP 1<sup>st</sup> marble  
(*Dependent Events*)

$$\frac{2}{10} * \frac{1}{9}$$

$$\frac{1}{5} * \frac{1}{9}$$

### Independent Events

The outcome of one event **does not** affect the outcome of the other.

If A and B are independent events then the probability of both occurring is


$$P(A \text{ and } B) = P(A) \times P(B)$$

### Dependent Events

The outcome of one event affects the outcome of the other.

If A and B are dependent events then the probability of both occurring is

$$P(A \text{ and } B) = P(A) \times P(B|A)$$



Probability of B given A

# Independent vs. Dependent Events



Using the bag of marbles on the left, what is the probability of pulling a black marble two times in a row?  $P(\text{black, black})$

When you put 1<sup>st</sup> marble back in  
(*Independent Events*)

$$\frac{2}{10} * \frac{2}{10}$$

$$\frac{1}{5} * \frac{1}{5} = \frac{1}{25}$$

When you KEEP 1<sup>st</sup> marble  
(*Dependent Events*)

$$\frac{2}{10} * \frac{1}{9}$$

$$\frac{1}{5} * \frac{1}{9}$$

$$P(A \text{ and } B) = P(A) \times P(B)$$

$$P(A \text{ and } B) = P(A) \times P(B | A)$$

Probability of B given A

# Marginal Probabilities



$\begin{cases} x = 1 & (\text{Rains}) \\ x = 0 & (\text{Doesn't rain}) \end{cases}$

$$\Pr(x = 1) = 0.6$$

$$\Pr(x = 0) = 0.4$$



$\begin{cases} y = 1 & (\text{Have umbrella}) \\ y = 0 & (\text{Don't have umbrella}) \end{cases}$

$$\Pr(y = 1) = 0.3$$

$$\Pr(y = 0) = 0.7$$

# Joint Probability



$\{x = 1$ (Rains)	$Pr(x = 1) = 0.6$
$\{x = 0$ (Doesn't rain)	$Pr(x = 0) = 0.4$
$\{y = 1$ (Have umbrella)	$Pr(y = 1) = 0.3$
$\{y = 0$ (Don't have umbrella)	$Pr(y = 0) = 0.7$

$$Pr(x = 0) = \sum_{y=0}^1 Pr(x=0, y)$$

$$= Pr(x=0, y=0) + Pr(x=0, y=1)$$

$$= 0.28 + 0.12 = 0.4$$

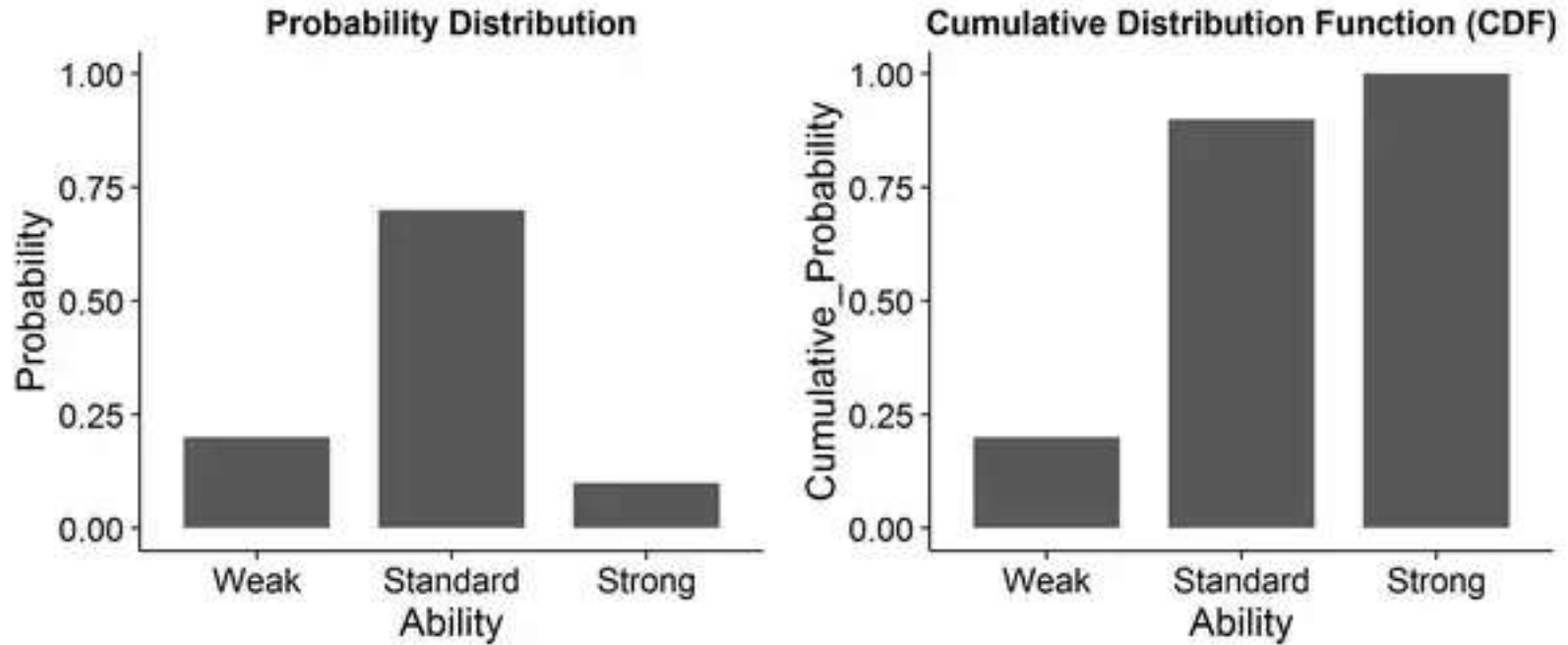
Case 1: Rains but you have an umbrella

$$\begin{aligned} Pr(x = 1, y = 1) &= Pr(x = 1) \times Pr(y = 1) \\ &= 0.6 \times 0.3 \\ &= 0.18 \end{aligned}$$

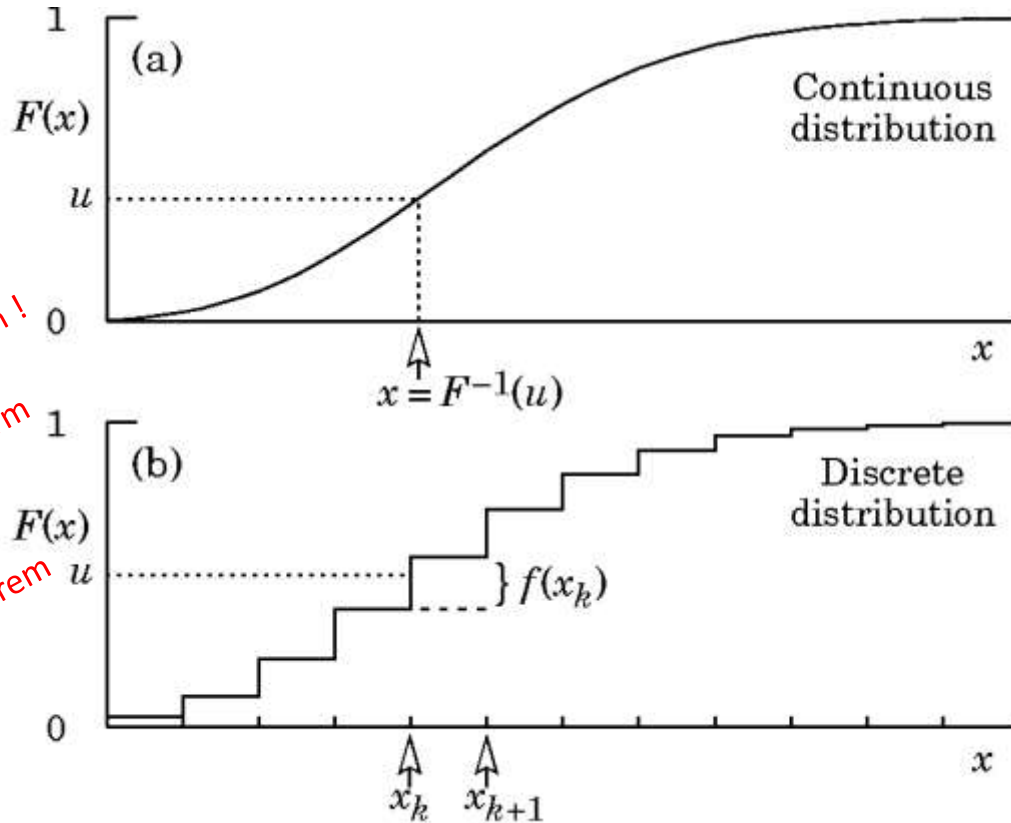
Case 2: Rains but you DON'T have an umbrella

$$\begin{aligned} Pr(x = 1, y = 0) &= Pr(x = 1) \times Pr(y = 0) \\ &= 0.6 \times 0.7 \\ &= 0.42 \end{aligned}$$

# Inverse Transform Sampling



# Inverse Transform Sampling



Does not work with Gaussian!  
CDF not in closed form.  
Need Box-Muller Transform  
Sample multiple times and  
Invoke Central Limit Theorem



23.08.2024

# Statistical Methods in AI (CS7.403)

## Lecture-7: Clustering (k-means)

Ravi Kiran ([ravi.kiran@iiit.ac.in](mailto:ravi.kiran@iiit.ac.in))

<https://ravika.github.io>



Center for Visual Information Technology (CVIT)

IIIT Hyderabad

# ML Tasks

```
graph TD; ML[ML Tasks] --> Predictive[Predictive]; ML --> Descriptive[Descriptive]; Predictive --> Classification[Classification]; Predictive --> Regression[Regression];
```

Predictive

Descriptive

Classification

Regression

ML Tasks

```
graph TD; A[ML Tasks] --> B[Predictive]; A --> C[Descriptive];
```

The diagram is a simple tree structure. At the top is a gray rectangular box containing the text 'ML Tasks'. A dark blue line descends from the center of this box and splits into two horizontal branches. The left branch leads to a solid red rectangular box containing the text 'Predictive'. The right branch leads to a purple rectangular box containing the text 'Descriptive'. This purple box is enclosed within a larger, dashed purple rectangular border, which has a subtle gray drop shadow.

Predictive

Descriptive

# Unsupervised Learning → Clustering

Group similar things e.g. images

[Goldberger et al.]



$C_1$



$C_2$



$C_3$



$C_4$



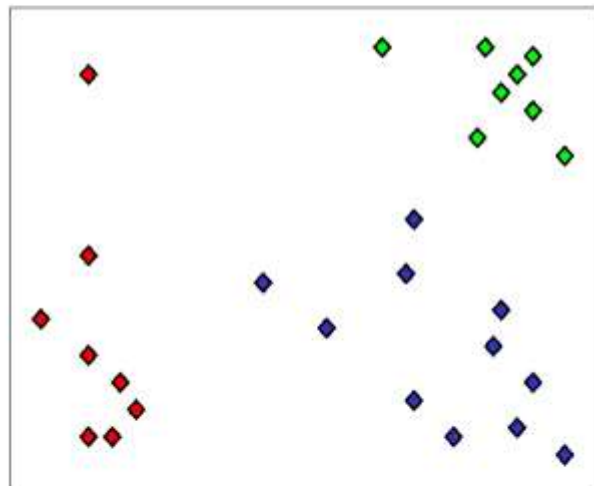
$C_5$

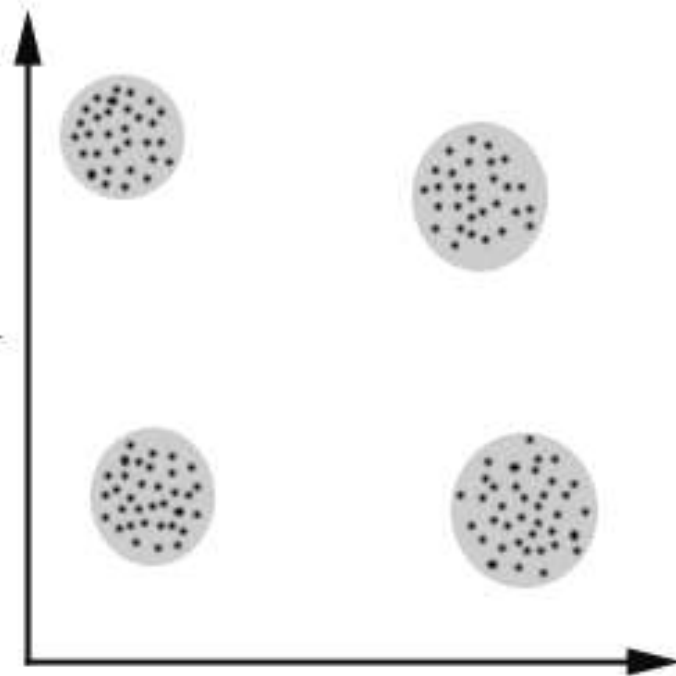
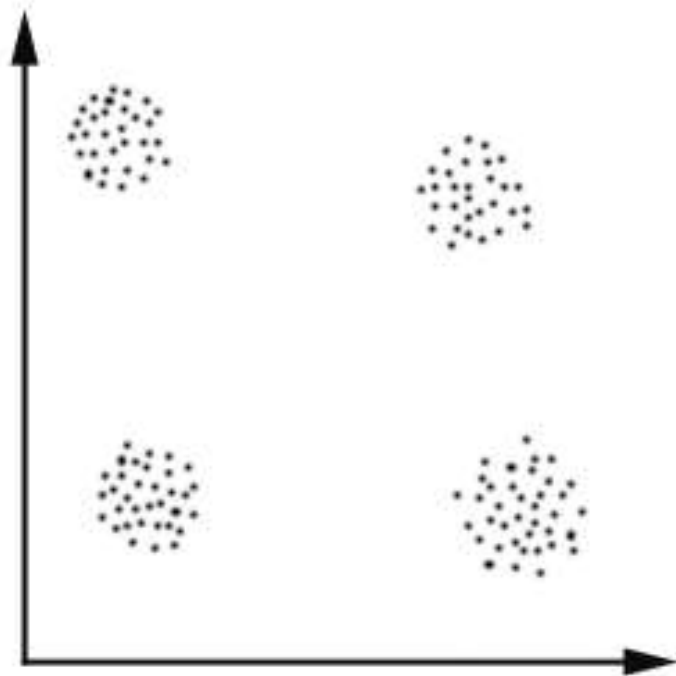


- Determine groups of people in image above
  - ▶ based on clothing styles
  - ▶ gender, age, etc

# What is Clustering?

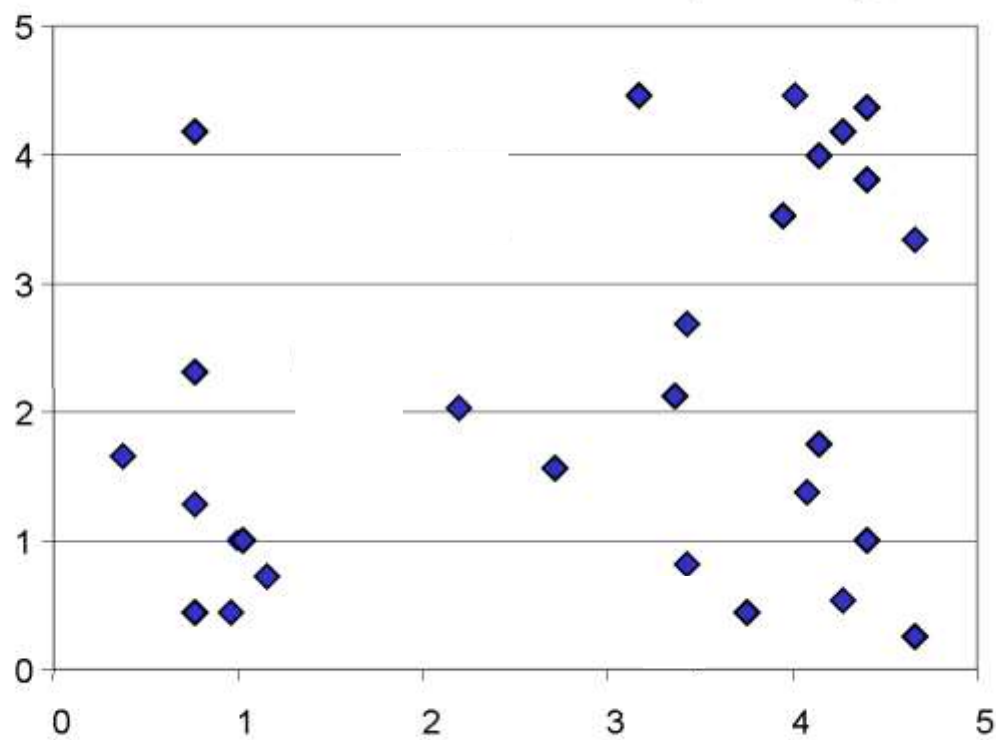
- Organizing data into *clusters* such that there is
  - high intra-cluster similarity
  - low inter-cluster similarity
- Informally, finding natural groupings among objects.





# K-means Clustering: Initialization

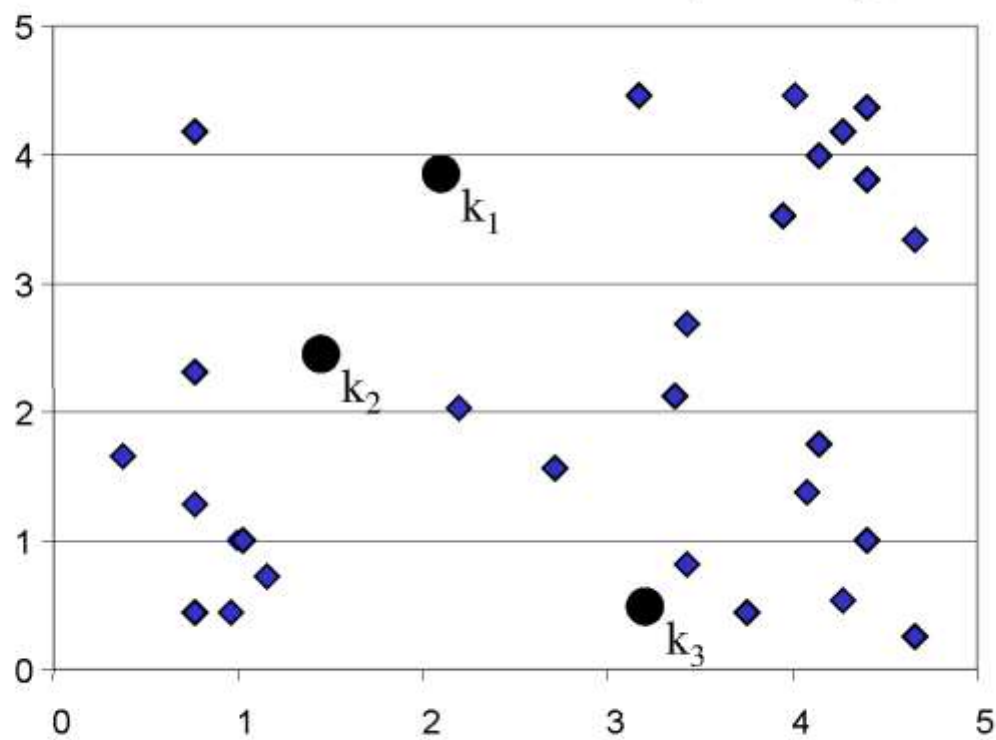
Decide  $K$ , and initialize  $K$  centers (randomly)





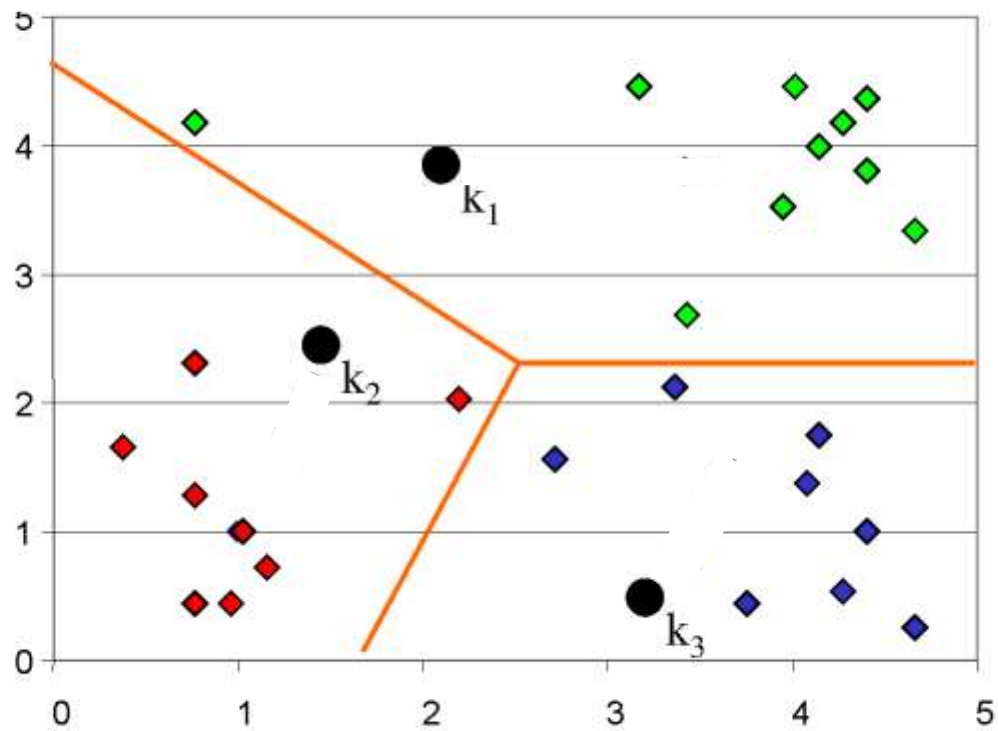
# K-means Clustering: Initialization

Decide  $K$ , and initialize  $K$  centers (randomly)



# K-means Clustering: Iteration 1

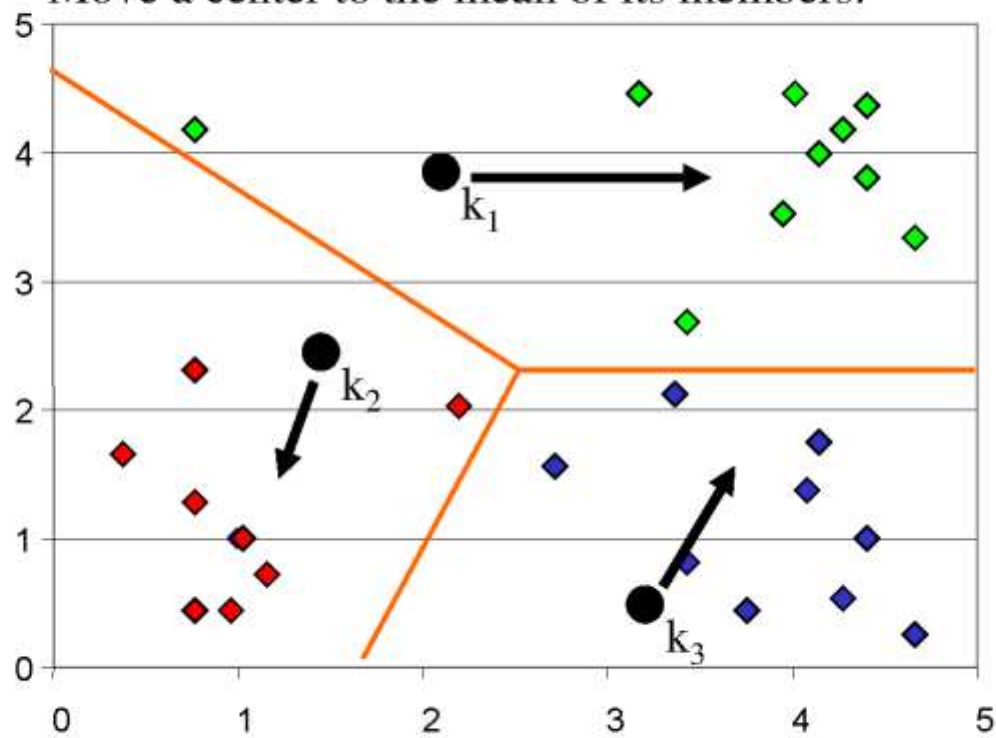
Assign all objects to the nearest center.



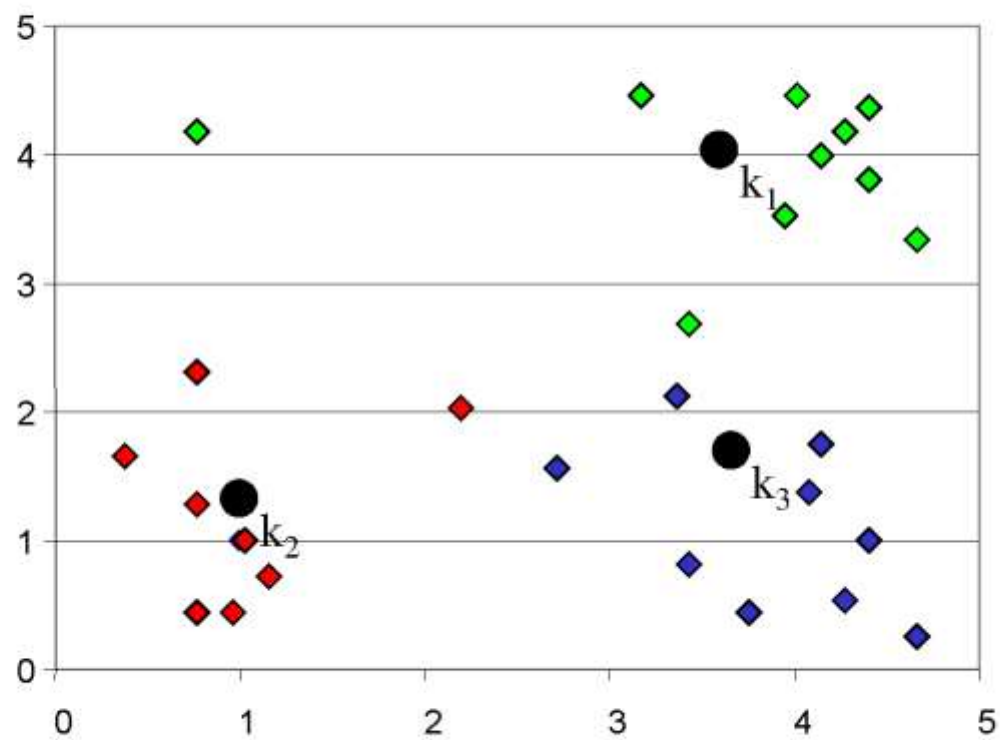
# K-means Clustering: Iteration 1

Assign all objects to the nearest center.

Move a center to the mean of its members.

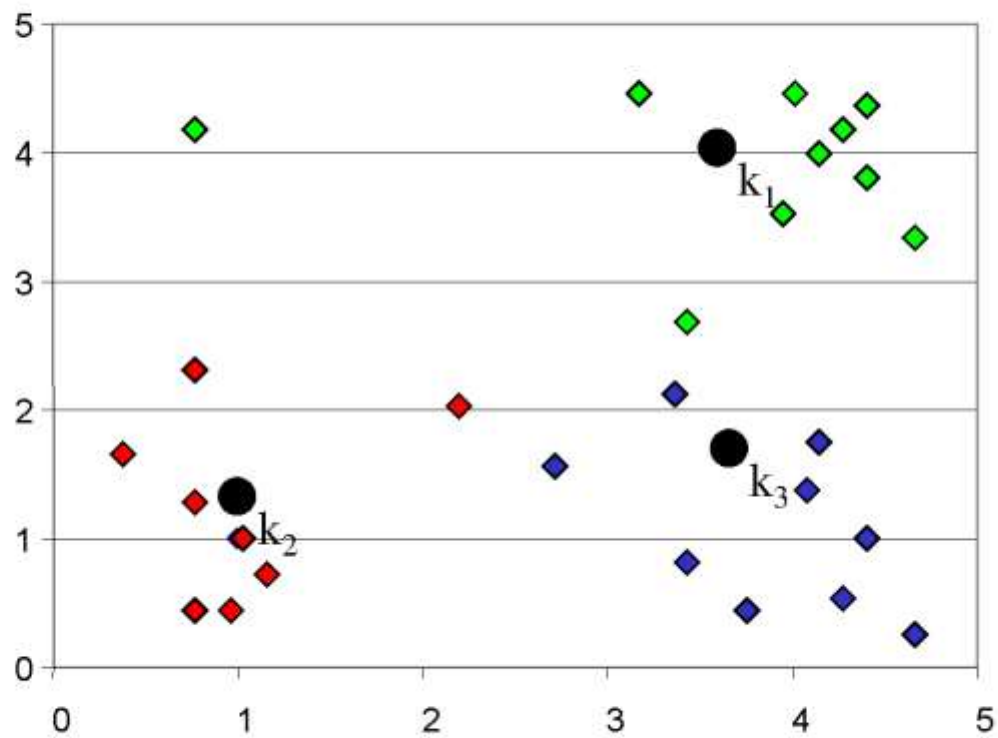


## K-means Clustering: Iteration 2



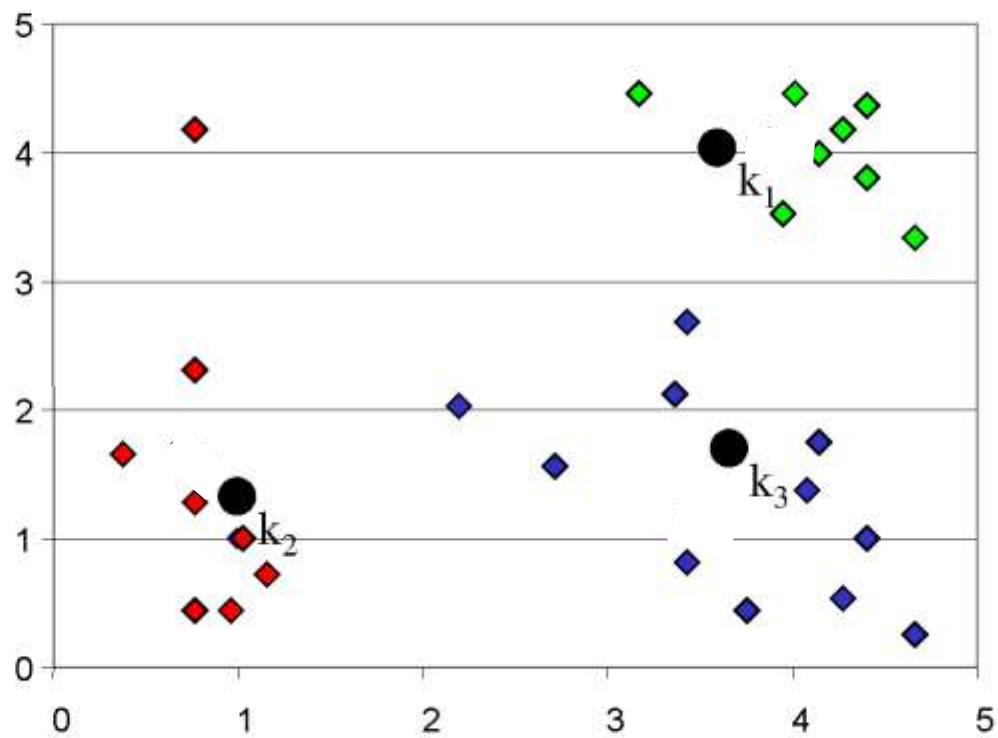
# K-means Clustering: Iteration 2

After moving centers, re-assign the objects...



# K-means Clustering: Iteration 2

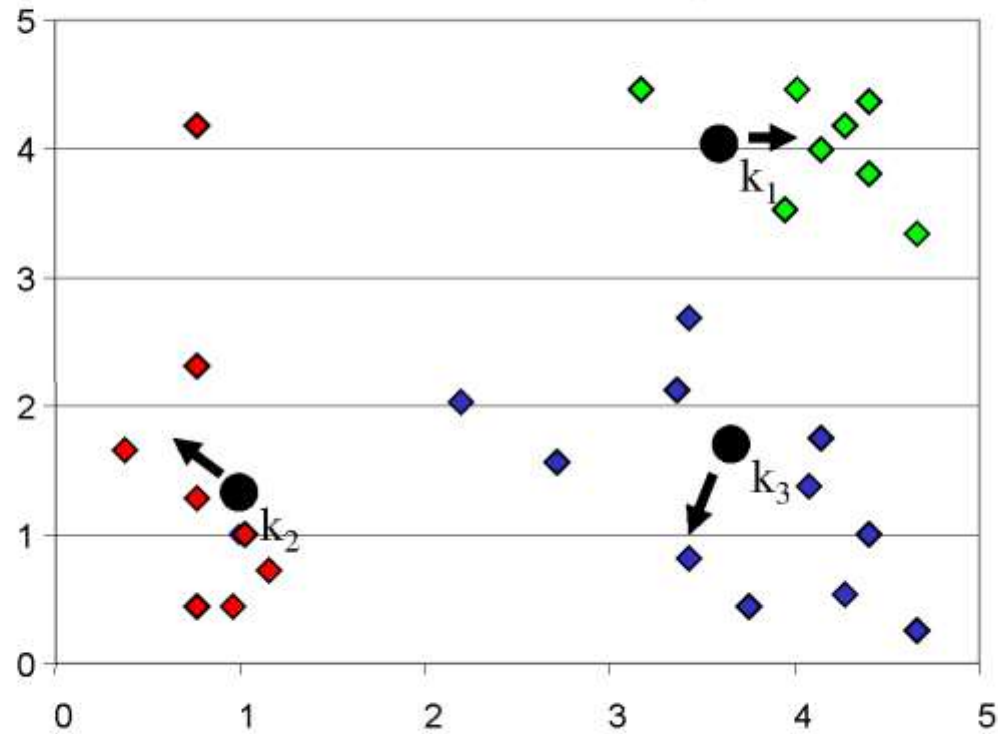
After moving centers, re-assign the objects to nearest centers.



# K-means Clustering: Iteration 2

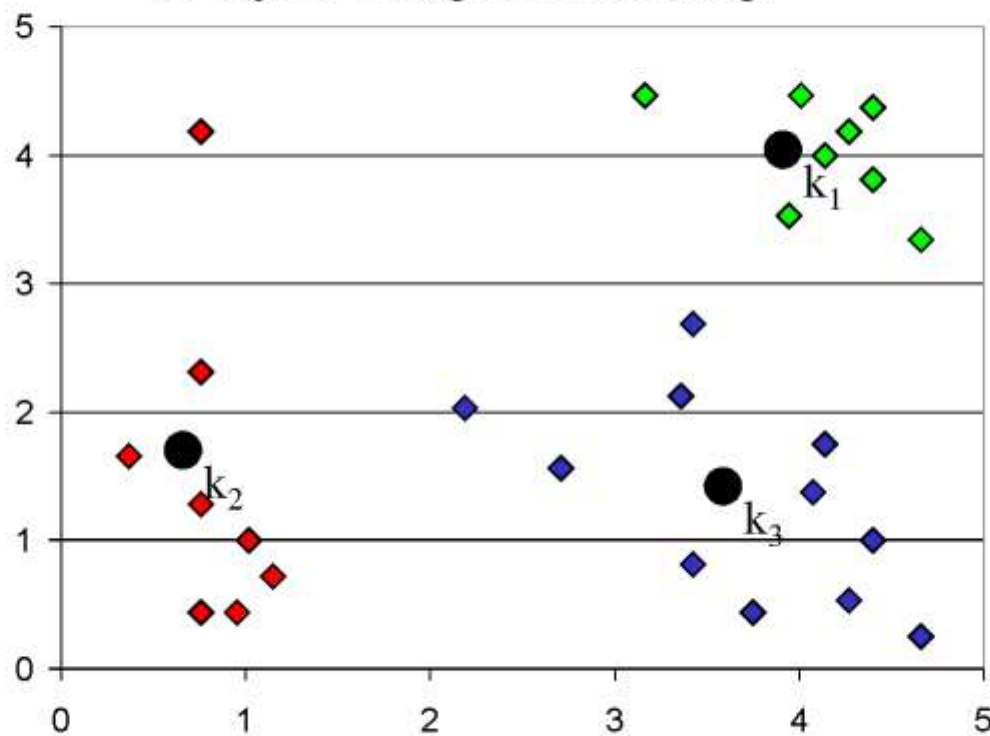
After moving centers, re-assign the objects to nearest centers.

Move a center to the mean of its new members.



# K-means Clustering: Finished!

Re-assign and move centers, until ...  
no objects changed membership.





$$\{x^{(1)}, \dots, x^{(m)}\} \quad x^{(i)} \in \mathbb{R}^n$$

The  $k$ -means clustering algorithm is as follows:

1. Initialize **cluster centroids**  $\mu_1, \mu_2, \dots, \mu_k \in \mathbb{R}^n$  randomly.

2. Repeat until convergence: {

For every  $i$ , set

$$c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2.$$

Assignment step: Assign each data point to the closest cluster

For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

Refitting step: Move each cluster center to the center of the data assigned to it

}

$$\{x^{(1)}, \dots, x^{(m)}\} \quad x^{(i)} \in \mathbb{R}^n$$

## EXPECTATION MAXIMIZATION

The  $k$ -means clustering algorithm is as follows:

1. Initialize **cluster centroids**  $\mu_1, \mu_2, \dots, \mu_k \in \mathbb{R}^n$  randomly.

2. Repeat until convergence: {

For every  $i$ , set

$$c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2.$$

E

Assignment step: Assign each data point to the closest cluster

For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

M

Refitting step: Move each cluster center to the center of the data assigned to it

}

$$\{x^{(1)}, \dots, x^{(m)}\} \quad x^{(i)} \in \mathbb{R}^n$$

The  $k$ -means clustering algorithm is as follows:

1. Initialize **cluster centroids**  $\mu_1, \mu_2, \dots, \mu_k \in \mathbb{R}^n$  randomly.

2. Repeat until convergence: {

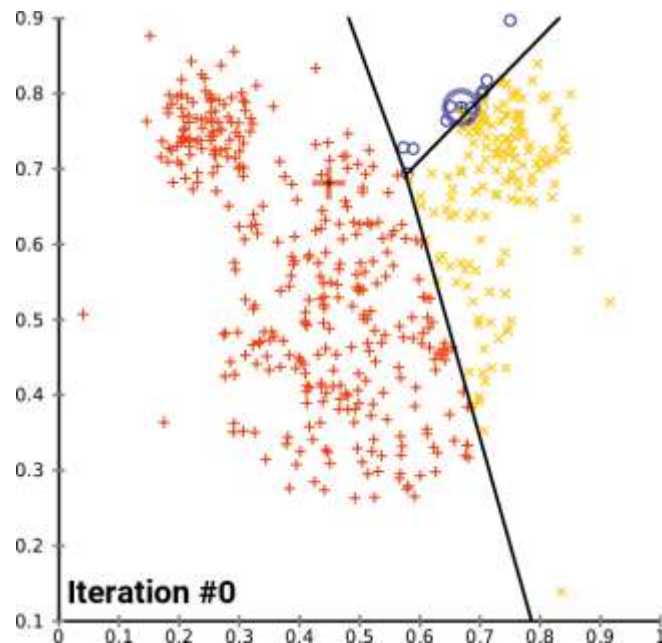
For every  $i$ , set

$$c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2.$$

For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

}



## Algorithm *k-means*

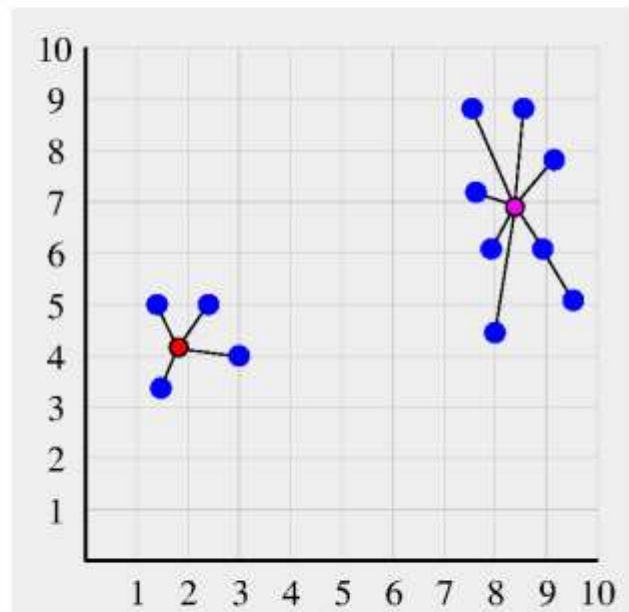
1. Decide on a value for  $K$ , the number of clusters.
2. Initialize the  $K$  cluster centers (randomly, if necessary).
3. Decide the class memberships of the  $N$  objects by assigning them to the nearest cluster center.
4. Re-estimate the  $K$  cluster centers, by assuming the memberships found above are correct.
5. Repeat 3 and 4 until none of the  $N$  objects changed membership in the last iteration.

## Algorithm *k-means*

1. Decide on a value for  $K$ , the number of clusters (usually between 2 and 10).
  - Use one of the distance / similarity functions we discussed earlier
2. Initialize the  $K$  cluster centers (e.g., choose  $K$  random objects or necessary).
3. Decide the class memberships of the  $N$  objects by assigning them to the nearest cluster center.
4. Re-estimate the  $K$  cluster centers, by assuming the memberships found above are correct.
5. Repeat 3 and 4 until none of the  $N$  objects changed membership in the last iteration.
  - Average / median of class members

# Why K-means Works

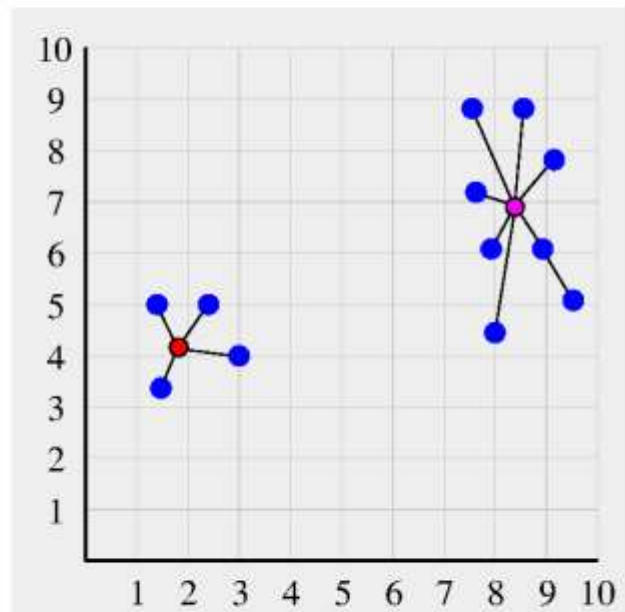
- What is a good partition?
- High intra-cluster similarity



# Why K-means Works

- What is a good partition?
- High intra-cluster similarity
- K-means optimizes

$$se = \sum_{k=1}^K \sum_{i=1}^{n_k} \|x_{ki} - \mu_k\|^2$$



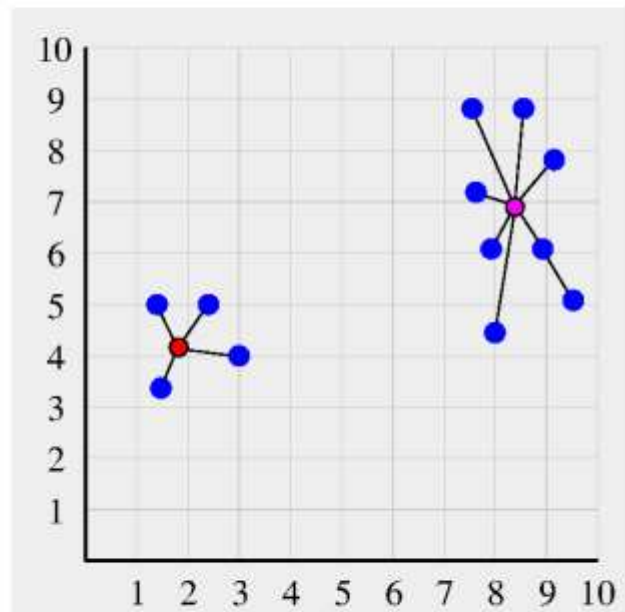
# Why K-means Works

- What is a good partition?
- High intra-cluster similarity
- K-means optimizes
  - the average distance to members of the same cluster

$$\sum_{k=1}^K \frac{1}{n_k} \sum_{i=1}^{n_k} \sum_{j=1}^{n_k} \|x_{ki} - x_{kj}\|^2$$

- which is twice the total distance to centers, also called squared error

$$se = \sum_{k=1}^K \sum_{i=1}^{n_k} \|x_{ki} - \mu_k\|^2$$





Repeat until convergence: {

For every  $i$ , set

$$c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2.$$

For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

}

$$\sum_{k=1}^K \sum_{i=1}^{n_k} \|x_{ki} - \mu_k\|^2$$

- Whenever an assignment is changed, the sum squared distances  $J$  of data points from their assigned cluster centers is reduced.

- Whenever an assignment is changed, the sum squared distances  $J$  of data points from their assigned cluster centers is reduced.

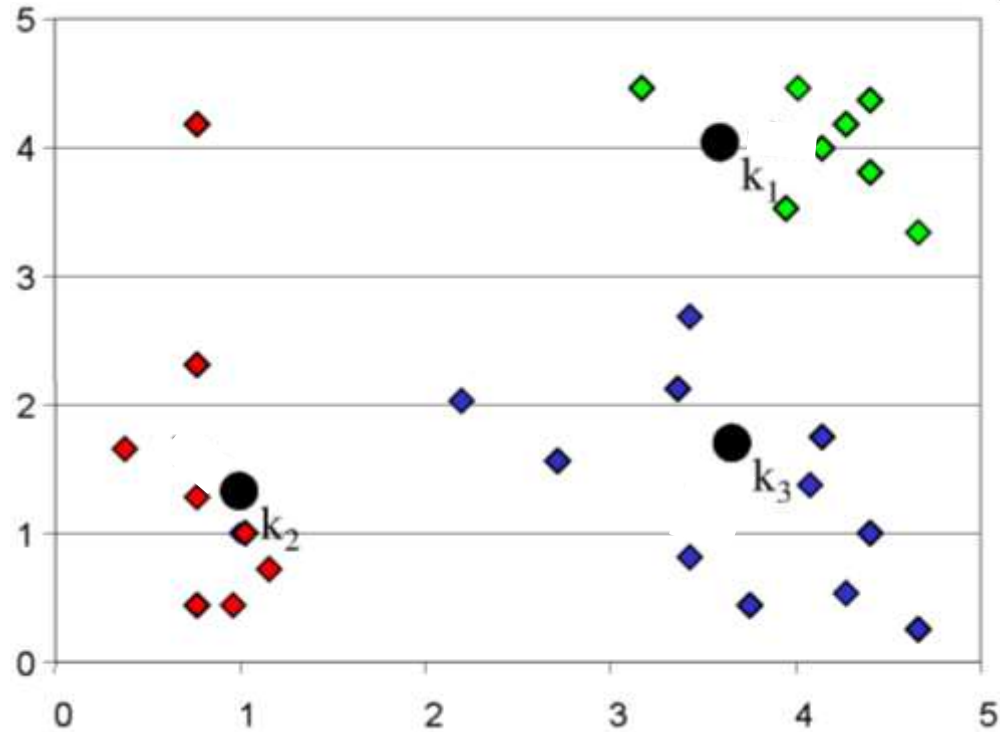
Repeat until convergence: {

For every  $i$ , set

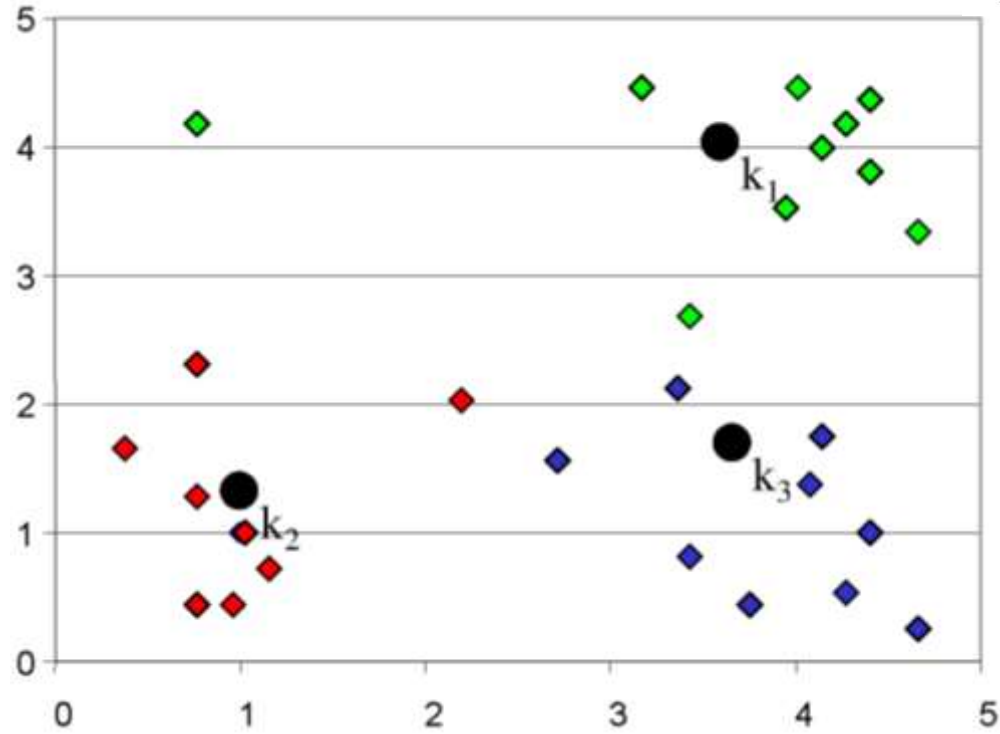
$$c^{(i)} := \arg \min_j ||x^{(i)} - \mu_j||^2.$$

For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$



- Whenever an assignment is changed, the sum squared distances  $J$  of data points from their assigned cluster centers is reduced.



Repeat until convergence: {

For every  $i$ , set

$$c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2.$$

For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

}

Repeat until convergence: {

For every  $i$ , set

$$c^{(i)} := \arg \min_j ||x^{(i)} - \mu_j||^2.$$

• Whenever an assignment is changed, the sum squared distances  $J$  of data points from their assigned cluster centers is reduced.

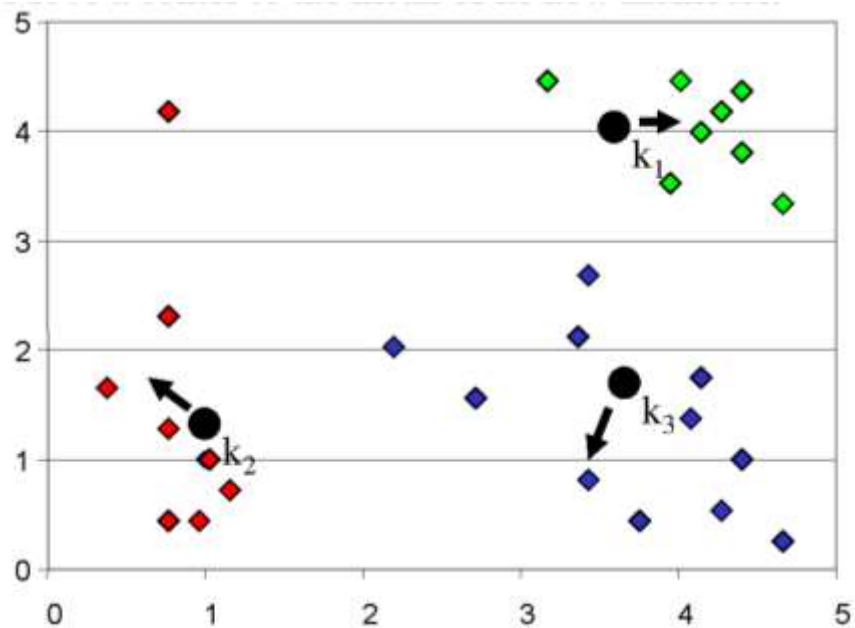
For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

• Whenever a cluster center is moved,  $J$  is reduced.

}

$$\sum_{k=1}^K \sum_{i=1}^{n_k} ||x_{ki} - \mu_k||^2$$



Repeat until convergence: {

For every  $i$ , set

$$c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2.$$

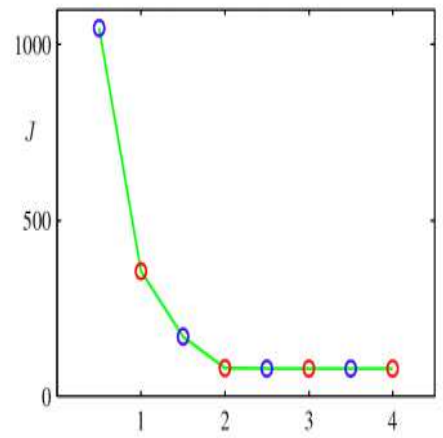
For each  $j$ , set

$$\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)} = j\}}.$$

}

$$\sum_{k=1}^K \sum_{i=1}^{n_k} \|x_{ki} - \mu_k\|^2$$

- Whenever an assignment is changed, the sum squared distances  $J$  of data points from their assigned cluster centers is reduced.
- Whenever a cluster center is moved,  $J$  is reduced.
- **Test for convergence:** If the assignments do not change in the assignment step, we have converged (to at least a local minimum).



- K-means cost function after each E step (blue) and M step (red). The algorithm has converged after the third M step

$K = 2$



$K = 3$



$K = 10$



Original image







- How would you modify k-means to get super pixels?