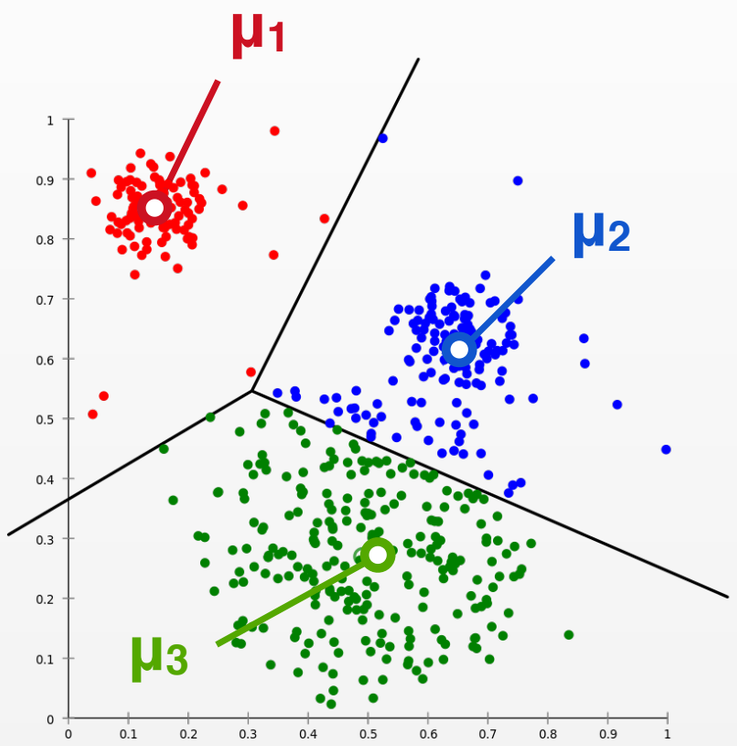
K-means Clustering

Initialization, Speed-ups and Limitations

Choice of Initialization

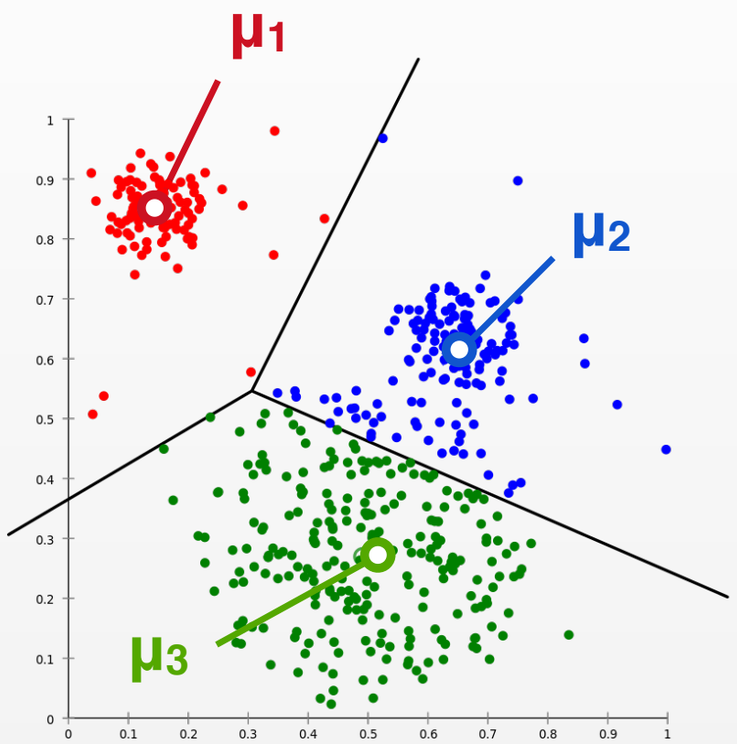


Loss: Sum of Squared Distances

$$L(\mu, z) = \sum_{k=1}^{K} \sum_{n=1}^{N} I[z_n = k] (x_n - \mu_k)^2$$

- Randomly initialize μ
- Alternate between two steps
  1. Minimize L(μ, z) with respect to z *(assign points to closest cluster)*
  2. Minimize L(μ, z) with respect to μ *(place clusters close to points)*

Choice of Initialization

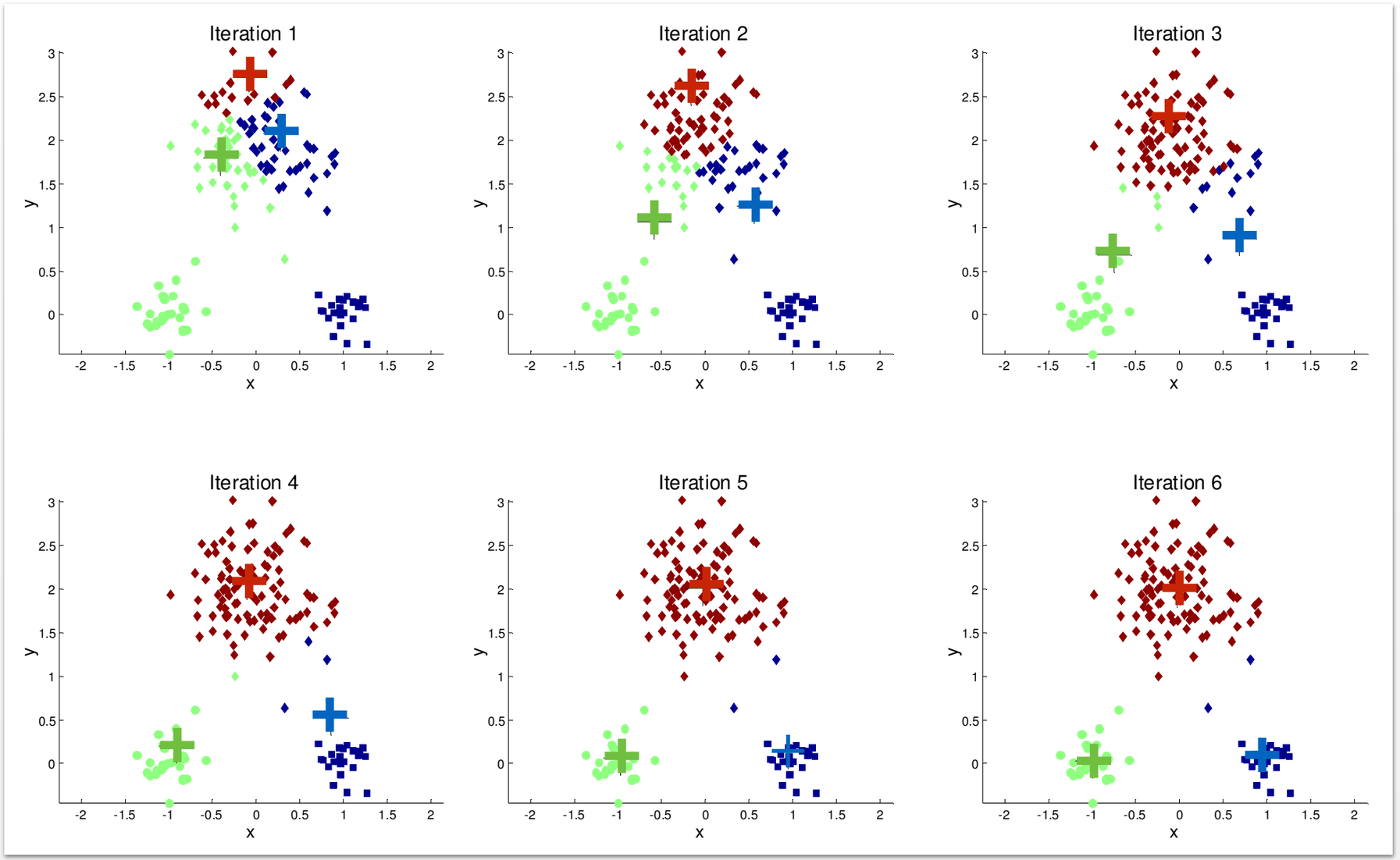


Loss: Sum of Squared Distances

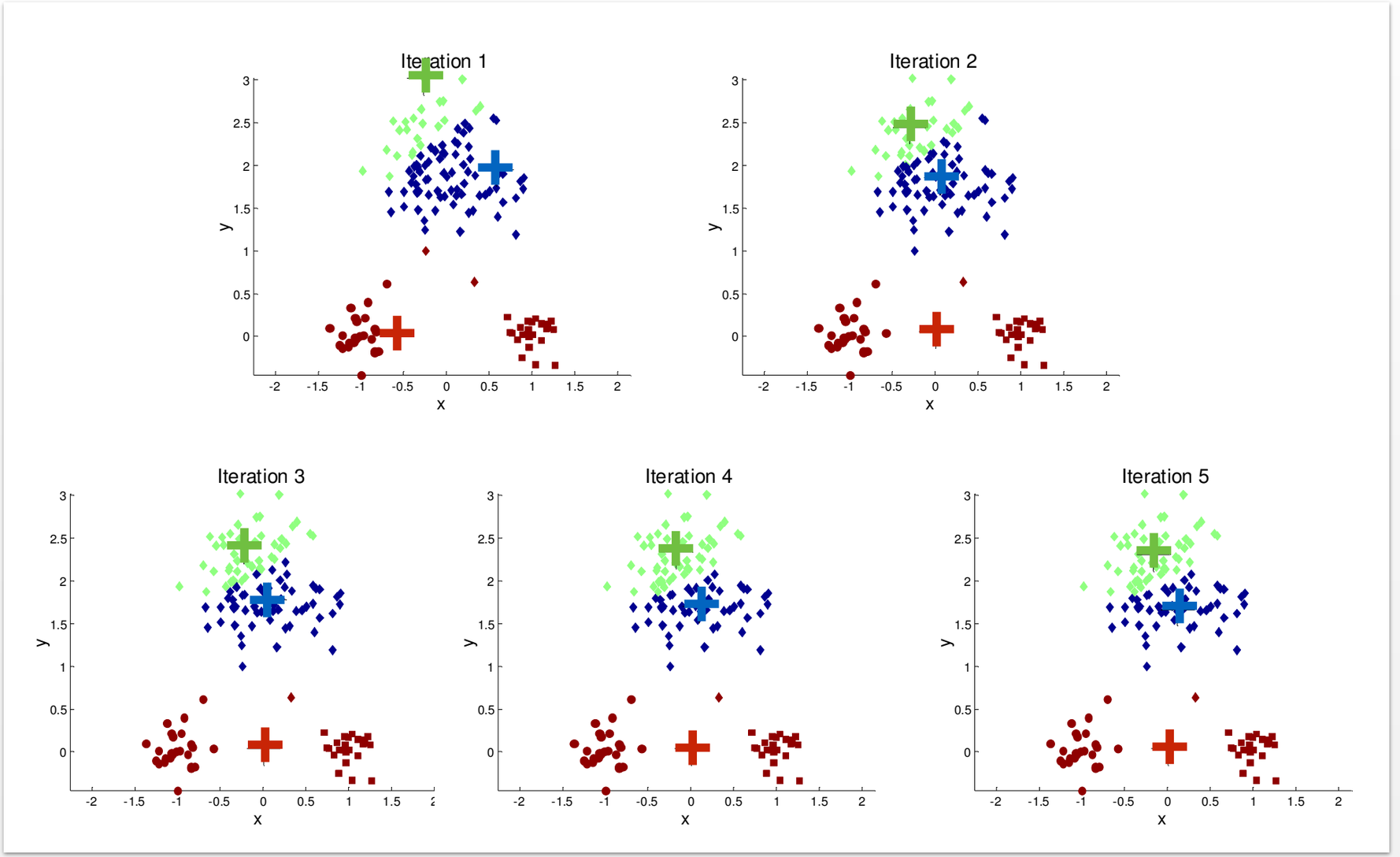
$$L(\mu, z) = \sum_{k=1}^{K} \sum_{n=1}^{N} I[z_n = k] (x_n - \mu_k)^2$$

- Randomly initialize μ *What is a good choice?*
- Alternate between two steps
  1. Minimize L(μ, z) with respect to z *(assign points to closest cluster)*
  2. Minimize L(μ, z) with respect to μ *(place clusters close to points)*

“Good” Initialization of Centroids



“Bad” Initialization of Centroids



Importance of Initial Centroids

Good initialization: Pick one point in each cluster

What is the chance of ***randomly*** selecting
one point from each of ***K*** clusters?
(assume each cluster has size ***n = N/K***)

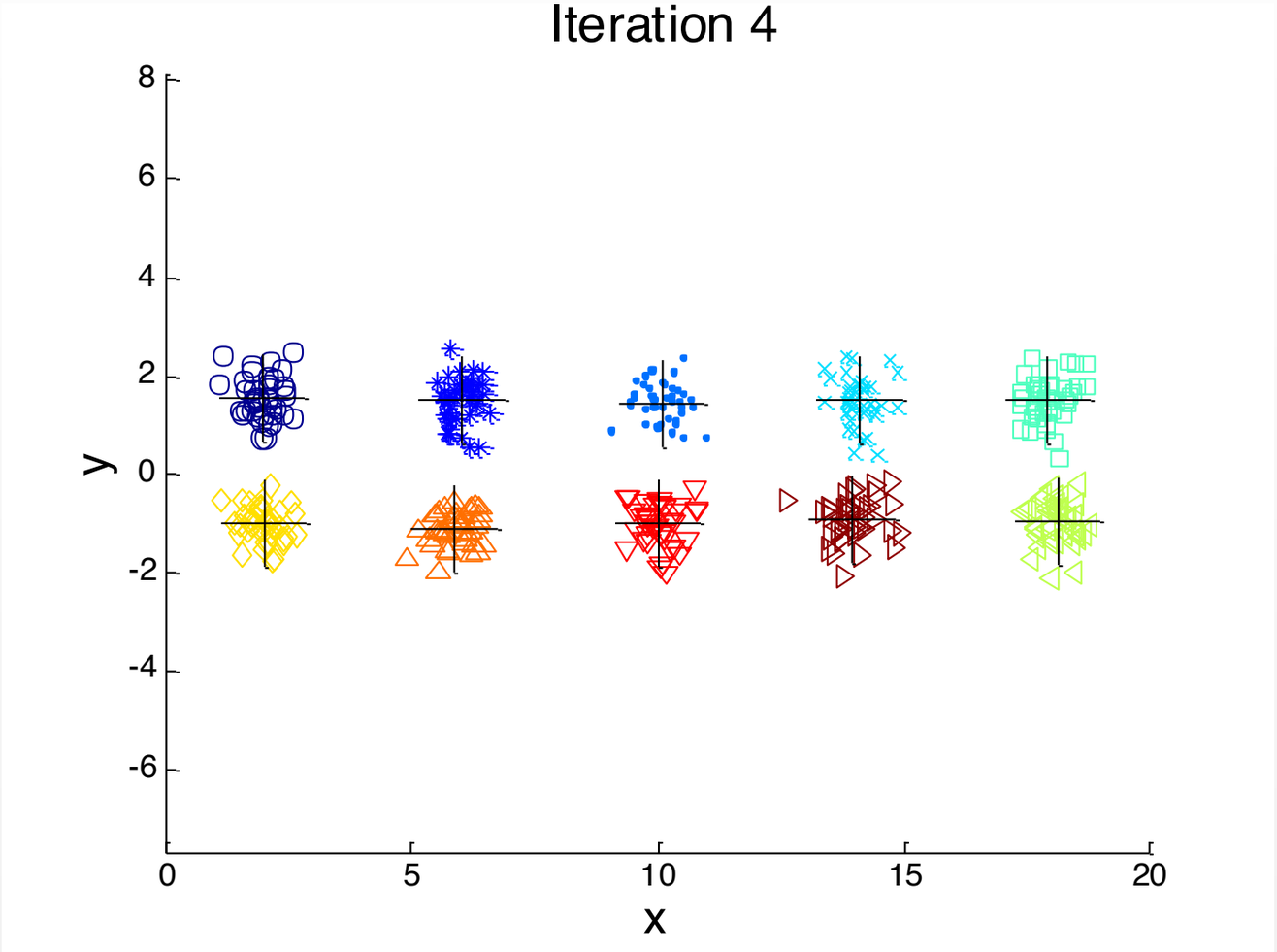
$$\frac{\text{ways to select one from each cluster}}{\text{ways to select K centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K} \approx \sqrt{2\pi K}\, e^{-K}$$

$\approx 10^{-4}$ for $K = 10$

$\approx 10^{-8}$ for $K = 20$

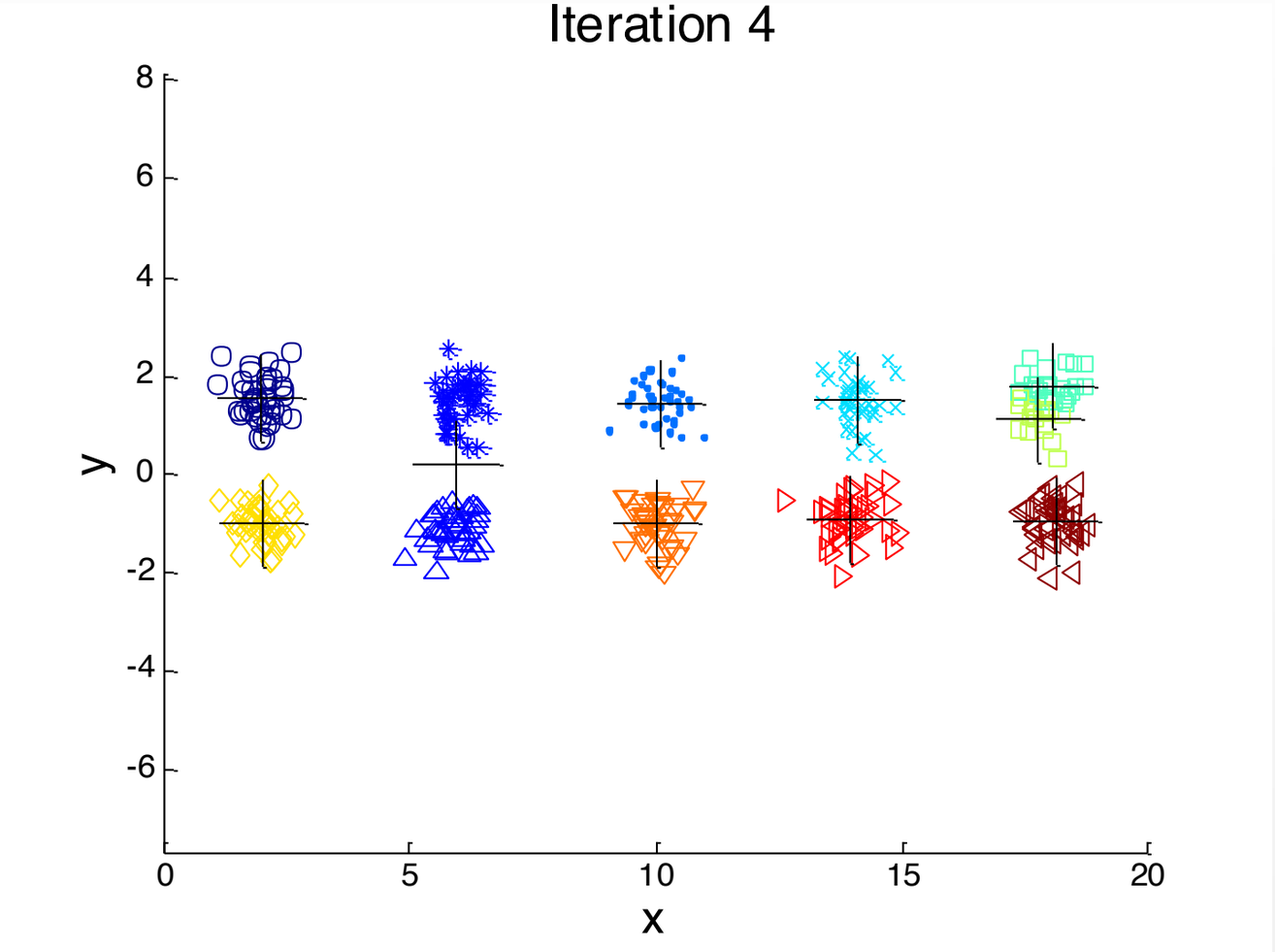
Implication: We will almost always have
multiple initial centroids in same cluster.

Example: 10 Clusters



5 pairs of clusters, two initial points in each pair

Example: 10 Clusters



Picking the initialization cluster centers: a significant issue

$\hat{z}$: cluster assignments returned by K-means, a local minimizer of the loss

z_{opt}: the global minimizer of the loss

It is the speed and simplicity of the k-means method that make it appealing, not its accuracy. Indeed, there are many natural examples for which the algorithm generates arbitrarily bad clustering (i.e., $L(\hat{z})/L(z_{opt})$ is unbounded even when N and K are fixed). This does not rely on an adversarial placement of the starting centers, and in particular, it can hold with high probability if the centers are chosen uniformly at random from the data points.

Arthur, David, and Sergei Vassilvitskii. *k-means++: The advantages of careful seeding*. Stanford, 2006.

Importance of Initial Centroids

Initialization tricks

- Use multiple restarts
  - Helps, but probability is not on your side
- Initialize with hierarchical clustering
- Select more than K points, keep most widely separated points.
- Bisecting K-means
- K-means++

Furthest first

- Pick first center to be the mean of the data

$$M_1 \leftarrow \{\mu_1\}$$

- For the subsequent centers iteratively pick the point whose distance to the closest center is largest.

$$\mu_{j+1} \leftarrow \text{argmax}_{x \in X}[D_{min}(x, M_j)]$$

$$M_{j+1} \rightarrow M_j \cup \{\mu_{j+1}\}$$

$D_{min}(x, M_j)$ distance of x to the closest center in M_j.

Problem: Outliers get chosen as centers.

M_j is the set of centroids at j^{th} step.

K-Means ++

1.Pick first center uniformly at random

$$M_1 \leftarrow \{\mu_1\}$$

2.For the subsequent centers iteratively pick a point $x \in X$ randomly with probability proportional to $D_{min}(x, M_j)$

$$\mu_{j+1} \leftarrow x \sim p(x) = \frac{D_{min}(x, M_j)^2}{\sum_{x \in X} D_{min}(x, M_j)^2}$$

$$M_{j+1} \rightarrow M_j \cup \{\mu_{j+1}\}$$

$D_{min}(x, M_j)$ distance of x to the closest center in M_j.

M_j is the set of centroids at j^{th} step.

Here the outliers still have a high probability of being selected compared to other points individually. However, the cumulative probability of points having moderately large distances lying in a dense region dominate the probability as a group.

Theoretical guarantees when using K-Means++

$$\mathbf{E}[L(\hat{z})] \leq (8 \log K + 2) L(z_{opt})$$

Arthur, David, and Sergei Vassilvitskii. *k-means++: The advantages of careful seeding*. Stanford, 2006.

k	Average ϕ		Minimum ϕ		Average T	
	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	135512	126433	119201	111611	0.14	0.13
25	48050.5	15.8313	25734.6	15.8313	1.69	0.26
50	5466.02	14.76	14.79	14.73	3.79	4.21

Table 2: Experimental results on the *Norm-25* dataset (n = 10000, d = 15)

k	Average ϕ		Minimum ϕ		Average T	
	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	7553.5	6151.2	6139.45	5631.99	0.12	0.05
25	3626.1	2064.9	2568.2	1988.76	0.19	0.09
50	2004.2	1133.7	1344	1088	0.27	0.17

Table 3: Experimental results on the *Cloud* dataset (n = 1024, d = 10)

k	Average ϕ		Minimum ϕ		Average T	
	k-means	k-means++	k-means	k-means++	k-means	k-means++
10	$3.45 \cdot 10^8$	$2.31 \cdot 10^7$	$3.25 \cdot 10^8$	$1.79 \cdot 10^7$	107.5	64.04
25	$3.15 \cdot 10^8$	$2.53 \cdot 10^6$	$3.1 \cdot 10^8$	$2.06 \cdot 10^6$	421.5	313.65
50	$3.08 \cdot 10^8$	$4.67 \cdot 10^5$	$3.08 \cdot 10^8$	$3.98 \cdot 10^5$	766.2	282.9

Table 4: Experimental results on the *Intrusion* dataset (n = 494019, d = 35)

Here ϕ is same as the loss

K-means Clustering

Speed-ups

K-means Clustering

K-means Algorithm

- *Randomly initialize means* [$\mu_1, \ldots, \mu_K$]
- Repeat until L(μ, z) unchanged
  - *Assign all points to **nearest** cluster*

$$z_n = \underset{k}{\operatorname{argmin}} \; ||\boldsymbol{x}_n - \boldsymbol{\mu}_k||^2$$

  - *Update cluster means*

$$\mu_k = \frac{1}{N_k} \sum_{n:\, z_n = k} \boldsymbol{x}_n$$

Finding new cluster assignments

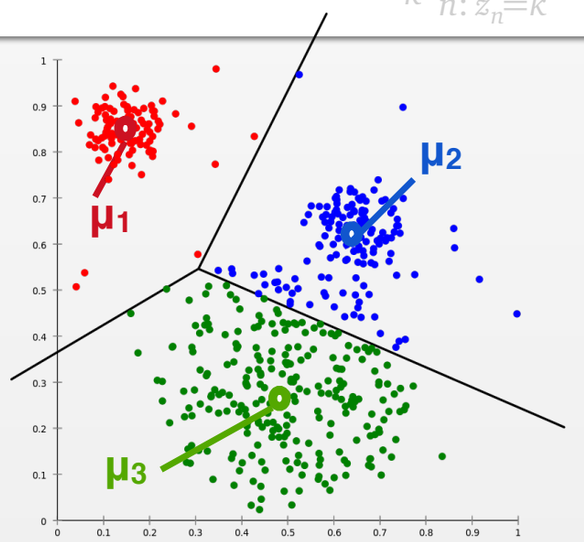
To compute all point-center distances

O(KND) computational complexity (per iteration) for *K* clusters, *N* points, and *D* features.

Updating the cluster centers

O(ND) computational complexity (per iteration)

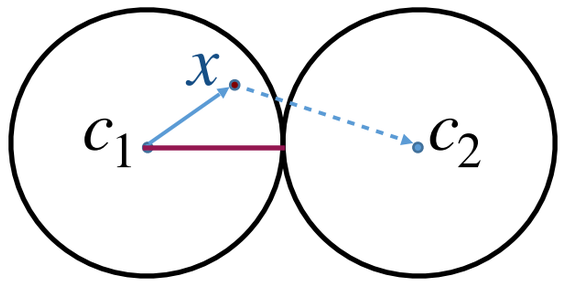
Can it be reduced further if only a few cluster assignments change?



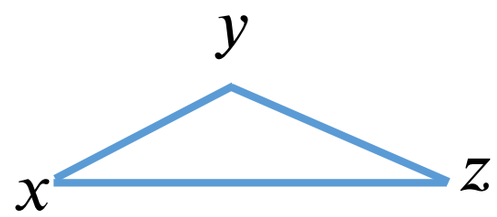
$O(NKD)$ per iteration is prohibitive in high dimensions and large K!

The core idea for cutting on distance computation

When updating the cluster assignments not all point-center distances need be computed



Exploit triangle inequality



$$d(x, z) \leq d(x, y) + d(y, z)$$

Also true when

$$d(x, c_1) \leq u \leq \frac{d(c_1, c_2)}{2}$$

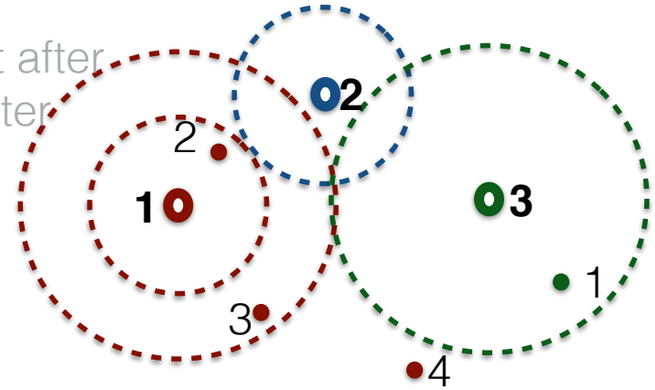
Upper bound for $d(x, c_1)$

$$d(x, c_1) \leq \frac{d(c_1, c_2)}{2} \Rightarrow d(x, c_1) \leq d(x, c_2)$$

If distance between x and center c_1 is relatively small compared to that between c_1 and another center c_2, the distance between x and c_2 need not be computed

Elkan's accelerated K-means

Before cluster assignments. Right after centers have moved. Closest center might not be the assigned center.



Conditions Checked:

1. $u(i) \leq s(a(i))$

   i^{th} point cluster assignment need not be changed. No distance involving the i^{th} point needs to be computed.

2. $u(i) \leq l(i,j)$ or $u(i) \leq \frac{d(c(a(i)), c(j))}{2}$

   i^{th} point cluster assignment might change, but it won't be assigned to center j. Distance from the j^{th} center need not be computed.

$a(i)$: contains the cluster index currently assigned to the i^{th} point.

$u(i)$: contains an upper bound to the distance of the i^{th} point to its current center

$l(i,j)$: contains a lower bound of the distance of the i^{th} point to the j^{th} center

$c(j)$: is the j^{th} center.

$s(j)$: is equal to half the distance of j^{th} center to its closest center

Bounding the distance of x from a center c after it moves to c^*

Distance computation: vector operation
Upper and lower bound: scalar operation

Lower bound

$$d(x, c^*) \geq \max(0,\ d(x, c) - d(c, c^*))$$
$$\geq \max(0,\ l - d(c, c^*))$$
$$= l^*$$

Old lower bound

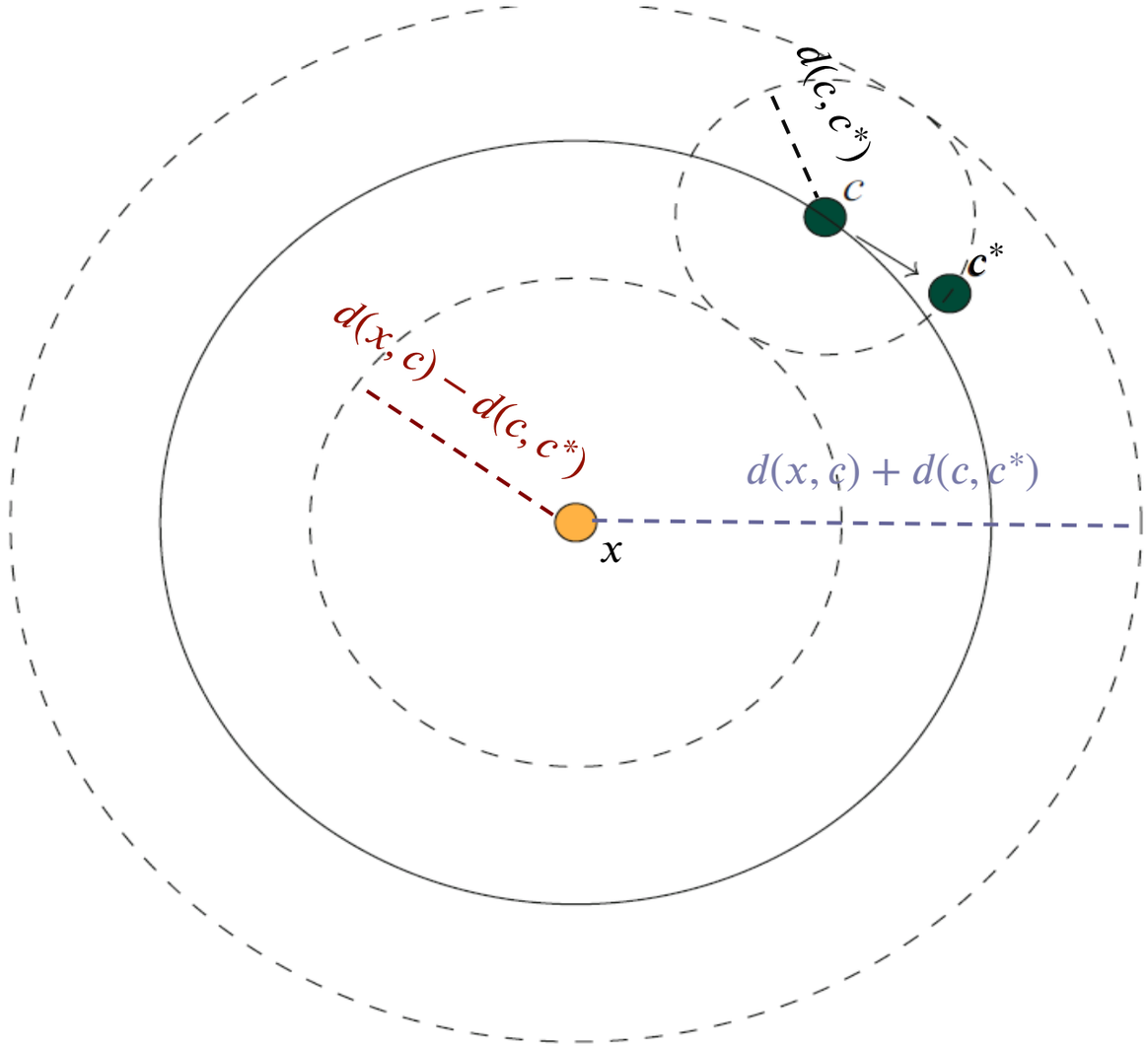
New lower bound

Upper bound

$$d(x, c^*) \leq d(x, c) + d(c, c^*)$$
$$\leq u + d(c, c^*)$$
$$= u^*$$

Old upper bound

New upper bound



Algorithm 3 Elkan's algorithm—using k lower bounds per point and k^2 center-center distances

```
procedure ELKAN(X, C)
    a(i) ← 1, u(i) ← ∞, ∀i ∈ N {Initialize invalid bounds, all in one cluster.}
    ℓ(i, j) ← 0, ∀i ∈ N, j ∈ K
    while not converged do
5:      compute ‖c(j) − c(j′)‖, ∀ j, j′ ∈ K
        compute s(j) ← min_{j′≠j} ‖c(j) − c(j′)‖/2, ∀ j ∈ K
        for all i ∈ N do
            if u(i) ≤ s(a(i)) then continue with next i
            r ← True
10:         for all j ∈ K do
                z ← max(ℓ(i, j), ‖c(a(i)) − c(j)‖/2)
                if j = a(i) or u(i) ≤ z then continue with next j
                if r then
                    u(i) ← ‖x(i) − c(a(i))‖
15:                 r ← False
                    if u(i) ≤ z then continue with next j
                ℓ(i, j) ← ‖x(i) − c(j)‖
                if ℓ(i, j) < u(i) then a(i) ← j
        for all j ∈ K do {Move the centers and track their movement}
20:     move c(j) to its new location
        let δ(j) be the distance moved by c(j)
        for all i ∈ N do {Update the upper and lower distance bounds}
            u(i) ← u(i) + δ(a(i))
            for all j ∈ K do
25:             ℓ(i, j) ← ℓ(i, j) − δ(j)
```

r: tells if the upper bound needs to be tightened.

Both upper bound and the lower bound are tight on this step.

$u(i) \leftarrow l(i,j)$

The upper bound should be updated at this step

$$\max\left(0, l(i,j) - \delta(j)\right)$$

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                z ← max(ℓ(i, j), ‖c(a(i)) − c(j)‖/2)
                if j = a(i) or u(i) ≤ z then continue with next j
                if r then
                    u(i) ← ‖x(i) − c(a(i))‖
15:                 r ← False
                    if u(i) ≤ z then continue with next j
                ℓ(i, j) ← ‖x(i) − c(j)‖
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            u(i) ← u(i) + δ(a(i))
            for all j ∈ K do
25:             ℓ(i, j) ← ℓ(i, j) − δ(j)
```

$$\max\left(0, l(i,j) - \delta(j)\right)$$

$O(K^2D)$

$O(N)$

$O(\alpha_1 NK)$

α_1 is the fraction of times the first condition is not satisfied

Since the bounds are loose in the first iteration, all distances will be computed: $O(NDK)$

$O(\alpha_1\alpha_2 NKD)$

α_2 is the fraction of times the second condition is not satisfied.

$O(KD)$

$O(NK)$

Running time of Elkan's K-means

Major computations

- Computing point-center distances
  - $O(NKD)$ in the first/first-few iteration.
  - $O(ND)$ over all later iterations combined. For most datasets with significant cluster structure.
- Computing pairwise center distances
  - $O(K^2DE)$
- Updating the lower bound
  - $O(NKE)$

Most points (in the core of the cluster) won't change cluster assignments after the first few iterations and will satisfy the pruning conditions. The more the clusters looks like gaussians, the more this true. This might no longer be true if the data lacks a cluster structure.

N: dataset size

K: number of clusters

D: number of dimensions

E: number of iterations

Results for Elkan

		$k = 3$	$k = 20$	$k = 100$
birch	iterations	17	38	56
	standard	5.100e+06	7.600e+07	5.600e+08
	fast	4.495e+05	1.085e+06	1.597e+06
	speedup	11.3	70.0	351
covtype	iterations	18	256	152
	standard	8.100e+06	7.680e+08	2.280e+09
	fast	9.416e+05	7.147e+06	7.353e+06
	speedup	8.60	107	310
kddcup	iterations	34	100	325
	standard	9.732e+06	1.908e+08	3.101e+09
	fast	6.179e+05	3.812e+06	1.005e+07
	speedup	15.4	50.1	309
mnist50	iterations	38	178	217
	standard	6.840e+06	2.136e+08	1.302e+09
	fast	1.573e+06	9.353e+06	3.159e+07
	speedup	4.35	22.8	41.2
mnist784	iterations	63	60	165
	standard	1.134e+07	7.200e+07	9.900e+08
	fast	1.625e+06	7.396e+06	3.055e+07
	speedup	6.98	9.73	32.4
random	iterations	52	33	18
	standard	1.560e+06	6.600e+06	1.800e+07
	fast	1.040e+06	3.020e+06	5.348e+06
	speedup	1.50	2.19	3.37

name	cardinality	dimensionality	description
birch	100000	2	10 by 10 grid of Gaussian clusters, DS1 in (Zhang et al., 1996)
covtype	150000	54	remote soil cover measurements, after (Moore, 2000)
kddcup	95413	56	KDD Cup 1998 data, un-normalized
mnist50	60000	50	random projection of NIST handwritten digit training data
mnist784	60000	784	original NIST handwritten digit training data
random	10000	1000	uniform random data

Table 2. Rows labeled "standard" and "fast" give the number of distance calculations performed by the unaccelerated k-means algorithm and by the new algorithm. Rows labeled "speedup" show how many times faster the new algorithm is, when the unit of measurement is distance calculations.

Limitations of Elkan

Storing and updating the lower bounds ($N \times K$ dimension) can be a bottleneck for large K

Can a smaller set of lower bounds be used?

Hamerly's accelerated K-means

Main difference from Elkan:

$l(i)$ instead of $l(i, j)$

Maintains one lower bound per point instead of K

$l(i)$: lower bound of the distance of the i^{th} point to the second closest centroid

Conditions Checked

$u(i) \leq s\left(a(i)\right)$ or $u(i) \leq l(i)$.

No distance involving the i^{th} point needs to be computed.

$O(N)$ instead of $O(N \times K)$ space for storing the lower bounds

Tradeoff

- Less memory for storing lower bounds.
- Fewer computations for updating lower bounds.
- However, there is less pruning and consequently more distance computation.

Algorithm 4 Hamerly's algorithm—using 1 lower bound per point

procedure HAMERLY(X, C)
  $a(i) \leftarrow 1, u(i) \leftarrow \infty, \ell(i) \leftarrow 0, \forall i \in N$ {Initialize invalid bounds, all in one cluster.}
  while not converged **do**
    compute $s(j) \leftarrow \min_{j' \neq j} \|c(j) - c(j')\|/2, \forall j \in K$
    for all $i \in N$ **do**
      $z \leftarrow \max(\ell(i), s(a(i)))$
      if $u(i) \leq z$ **then** continue with next i
      $u(i) \leftarrow \|x(i) - c(a(i))\|$ {Tighten the upper bound}
      if $u(i) \leq z$ **then** continue with next i
      Find $c(j)$ and $c(j')$, the two closest centers to $x(i)$, as well as the distances to each.
      if $j \neq a(i)$ **then**
        $a(i) \leftarrow j$
        $u(i) \leftarrow \|x(i) - c(a(i))\|$
      $\ell(i) \leftarrow \|x(i) - c(j')\|$
    for all $j \in K$ **do** {Move the centers and track their movement}
      move $c(j)$ to its new location
      let $\delta(j)$ be the distance moved by $c(j)$
    $\delta' \leftarrow \max_{j \in K} \delta(j)$
    for all $i \in N$ **do** {Update the upper and lower distance bounds}
      $u(i) \leftarrow u(i) + \delta(a(i))$
      $\ell(i) \leftarrow \ell(i) - \delta'$ $\max(0, l(i) - \delta')$

$l(i)$ by definition is also a lower bound to the distances to other centers, except the closest one.

δ' ensures that if the second closest cluster changes the lower bound is still valid.

Dataset		Total user CPU Seconds (User CPU seconds per iteration)							
		$k = 3$		$k = 20$		$k = 100$		$k = 500$	
uniform random	iterations	44		227		298		710	
$n = 1250000$	lloyd	4.0	(0.058)	61.4	(0.264)	320.2	(1.070)	3486.9	(4.909)
$d = 2$	kd-tree	3.5	(**0.006**)	**11.8**	(**0.035**)	34.6	(0.102)	338.8	(0.471)
	elkan	7.2	(0.133)	75.2	(0.325)	353.1	(1.180)	2771.8	(3.902)
	hamerly	**2.7**	(0.031)	14.6	(0.058)	**28.2**	(**0.090**)	**204.2**	(**0.286**)
uniform random	iterations	121		353		312		1405	
$n = 1250000$	lloyd	21.8	(0.134)	178.9	(0.491)	660.7	(2.100)	13854.4	(9.857)
$d = 8$	kd-tree	117.5	(0.886)	622.6	(1.740)	2390.8	(7.633)	46731.5	(33.254)
	elkan	14.1	(0.071)	130.6	(0.354)	591.8	(1.879)	11827.9	(8.414)
	hamerly	**10.9**	(**0.045**)	**40.4**	(**0.099**)	**169.8**	(**0.527**)	**1395.6**	(**0.989**)
uniform random	iterations	137		4120		2096		2408	
$n = 1250000$	lloyd	66.4	(0.323)	5479.5	(1.325)	12543.8	(5.974)	68967.3	(28.632)
$d = 32$	kd-tree	208.4	(1.324)	29719.6	(7.207)	74181.3	(35.380)	425513.0	(176.697)
	elkan	48.1	(0.189)	1370.1	(0.327)	2624.9	(1.242)	14245.9	(5.907)
	hamerly	**46.9**	(**0.180**)	**446.4**	(**0.103**)	**1238.9**	(**0.581**)	**9886.9**	(**4.097**)
birch	iterations	52		179		110		99	
$n = 100000$	lloyd	0.53	(0.004)	4.60	(0.024)	11.80	(0.104)	48.87	(0.490)
$d = 2$	kd-tree	**0.41**	(<**0.001**)	0.96	(**0.003**)	2.67	(0.021)	17.68	(0.173)
	elkan	0.58	(0.005)	4.35	(0.023)	11.80	(0.104)	54.28	(0.545)
	hamerly	0.44	(0.002)	**0.90**	(**0.003**)	**1.86**	(**0.014**)	**7.81**	(**0.075**)
covtype	iterations	19		204		320		111	
$n = 150000$	lloyd	3.52	(0.048)	48.02	(0.222)	322.25	(0.999)	564.05	(5.058)
$d = 54$	kd-tree	6.65	(0.205)	266.65	(1.293)	2014.03	(6.285)	3303.27	(29.734)
	elkan	3.07	(0.022)	11.58	(0.044)	70.45	(0.212)	**152.15**	(**1.347**)
	hamerly	**2.95**	(**0.019**)	**7.40**	(**0.024**)	**42.83**	(**0.126**)	169.53	(1.505)
kddcup	iterations	39		55		169		142	
$n = 95412$	lloyd	4.74	(0.032)	12.35	(0.159)	116.63	(0.669)	464.22	(3.244)
$d = 56$	kd-tree	9.68	(0.156)	58.55	(0.996)	839.31	(4.945)	3349.47	(23.562)
	elkan	4.13	(0.012)	6.24	(0.049)	32.27	(0.169)	**132.39**	(**0.907**)
	hamerly	**3.95**	(**0.011**)	**5.87**	(**0.042**)	**28.39**	(**0.147**)	197.26	(1.364)
mnist50	iterations	37		249		190		81	
$n = 60000$	lloyd	2.92	(0.018)	23.18	(0.084)	75.82	(0.387)	162.09	(1.974)
$d = 50$	kd-tree	4.90	(0.069)	100.09	(0.393)	371.57	(1.943)	794.51	(9.780)
	elkan	2.42	(0.005)	7.02	(0.019)	**21.58**	(**0.101**)	**55.61**	(**0.660**)
	hamerly	**2.41**	(**0.004**)	**4.54**	(**0.009**)	21.95	(0.104)	77.34	(0.928)

Table 3: These results show the fraction of times that each algorithm was able to skip the innermost loop on data of different dimensions (values closer to 1 are better). These results are averaged over runs using k = 3, 20, 100, and 500 (one run for each k). The randX datasets are uniform random hypercube data with X dimensions.

dataset	rand2	rand8	rand32	rand128
elkan	0.56	0.01	0.00	0.00
hamerly	0.97	0.88	0.91	0.83

dataset	birch	covtype	kddcup	mnist50
elkan	0.52	0.34	0.18	0.22
hamerly	0.94	0.89	0.82	0.82

Memory requirements

		Megabytes			
Dataset	Algorithm	k=3	k=20	k=100	k=500
uniform	lloyd	7.5	7.5	7.5	7.5
random	kd-tree	32.1	32.1	32.1	32.1
n=1.25M	elkan	19.8	60.3	251.0	1205.2
d=2	hamerly	14.7	14.7	14.7	14.7
uniform	lloyd	21.9	21.9	21.9	21.9
random	kd-tree	54.8	54.8	54.8	54.8
n=1.25M	elkan	34.1	74.6	265.3	1219.5
d=8	hamerly	29.0	29.0	29.0	29.0
uniform	lloyd	79.1	79.1	79.1	79.1
random	kd-tree	145.2	145.2	145.2	145.3
n=1.25M	elkan	91.3	131.8	322.6	1276.8
d=32	hamerly	86.2	86.2	86.2	86.3
birch	lloyd	1.4	1.1	1.1	1.3
n=100K	kd-tree	2.9	2.9	2.8	2.7
d=2	elkan	2.1	5.2	20.6	97.3
	hamerly	1.5	1.7	1.6	1.5
covtype	lloyd	16.2	16.2	16.1	16.4
n=150K	kd-tree	27.2	27.2	27.2	27.3
d=54	elkan	17.4	22.5	45.3	160.4
	hamerly	17.0	17.0	16.8	17.2
kddcup	lloyd	10.9	10.8	11.1	11.2
n=95412	kd-tree	18.8	18.9	19.1	19.0
d=56	elkan	11.9	15.1	29.6	103.1
	hamerly	11.6	11.6	11.3	11.7
mnist50	lloyd	6.3	6.6	6.4	6.8
n=60K	kd-tree	10.5	10.4	10.6	10.7
d=50	elkan	7.0	9.1	18.4	64.8
	hamerly	6.9	6.9	6.9	6.8

Summary

- For moderate D (< 50) and K(< 100), Hamerly is well-suited (has smaller time and memory footprint).
- Large D (greater than 50), Elkan might be better (has smaller time footprint, in spite of large memory requirements).

Speed up with an approximate algorithm

Mini-batch K-means

Web-scale k-means **clustering**
D Sculley - Proceedings of the 19th international conference on …, 2010 - dl.acm.org
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Web-Scale K-Means Clustering

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Unsupervised clustering is an important task in a range of web-based applications, including grouping search results, near-duplicate detection, and news aggregation to name but a few. Lloyd's classic k-means algorithm remains a popular choice for real-world clustering tasks [6]. However, the standard batch algorithm is slow for large data sets. Even optimized batch k-means variants exploiting triangle inequality [3] cannot cheaply meet the latency needs of user-facing applications when clustering results on large data sets are required in a fraction of a second.

This paper proposes a mini-batch k-means variant that yields excellent clustering results with low computation cost on large data sets. We also give methods for learning sparse cluster centers that reduce storage and network cost.

2. MINI-BATCH K-MEANS

The k-means optimization problem is to find the set C of cluster centers $\mathbf{c} \in \mathbb{R}^m$, with $|C| = k$, to minimize over a set X of examples $\mathbf{x} \in \mathbb{R}^m$ the following objective function:

$$\min \sum_{\mathbf{x} \in X} ||f(C, \mathbf{x}) - \mathbf{x}||^2$$

Here, $f(C, \mathbf{x})$ returns the nearest cluster center $\mathbf{c} \in C$ to $\mathbf{x}$ using Euclidean distance. It is well known that although this problem is NP-hard in general, gradient descent methods converge to a local optimum when seeded with an initial set of k examples drawn uniformly at random from X [1].

The classic batch k-means algorithm is expensive for large data sets, requiring $O(kns)$ computation time where n is the number of examples and s is the maximum number of non-zero elements in any example vector. Bottou and Bengio proposed an online, stochastic gradient descent (SGD) variant of this computed a gradient descent step on one example at a time [1]. While SGD converges quickly on large data sets, it finds lower quality solutions than the batch algorithm due to stochastic noise [1].

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    end for
end for
```

We propose the use of mini-batch optimization for k-means clustering, given in Algorithm 1. The motivation behind this method is that mini-batches tend to have lower stochastic noise than individual examples in SGD (allowing convergence to better solutions) but do not suffer increased computational cost when data sets grow large with redundant examples. We use per-center learning rates for fast convergence, in the manner of [1]; convergence properties follow closely from this prior result [1].

Experiments. We tested the mini-batch k-means against both Lloyd's batch k-means [6] and the SGD variant of [1]. We used the standard `RCV1` collection of documents [4] for our experiments. To assess performance at scale, the set of 781,265 examples were used for training and the remaining 23,149 examples for testing. On each trial, the same random initial cluster centers were used for each method. We evaluated the learned cluster centers using the k-means objective function on the held-out test set; we report fractional error from the best value found by the batch algorithm run to convergence. We set the mini-batch b to 1000 based on separate initial tests; results were robust for a range of b.

The results (Fig. 1) show a clear win for mini-batch k-means. The mini-batch method converged to a near optimal value several orders of magnitude faster than the full batch method, and also achieved significantly better solutions than SGD. Additional experiments (omitted for space) showed that mini-batch k-means is several times faster on large data sets than batch k-means exploiting triangle inequality [3].

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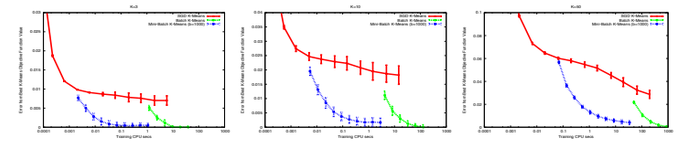

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Sparsity may be induced in gradient descent using the projected-gradient method, projecting a given $\mathbf{v}$ to the nearest point in an $L1$-ball of radius λ after each update [2]. Thus, for mini-batch k-means we achieve sparsity by performing an $L1$-ball projection on each cluster center $\mathbf{c}$ after each mini-batch iteration.

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```
Given: ε tolerance, L1-ball radius λ, vector c ∈ R^m
if ||c||_1 ≤ λ + ε then exit
upper ← ||c||_∞ ; lower ← 0 ; current ← ||c||_1
while current > λ(1 + ε) or current < λ do
    θ ← (upper+lower)/2.0        // Get L1 value for this θ
    current ← Σ_{c_i ≠ 0} max(0, |c_i| − θ)
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for i = 1 to m do
    c_i ← sign(c_i) * max(0, |c_i| − θ) // Do the projection
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Fast $L1$ Projections. Applying $L1$ constraints to k-means clustering has been studied in forthcoming work by Witten and Tibshirani [5]. There, a hard $L1$ constraint was applied in the full batch setting of maximizing between-cluster distance for k-means (rather than minimizing the k-means objective function directly); the work did not discuss how to perform this projection efficiently.

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full batch	-	200,319	0 (baseline)	133.96
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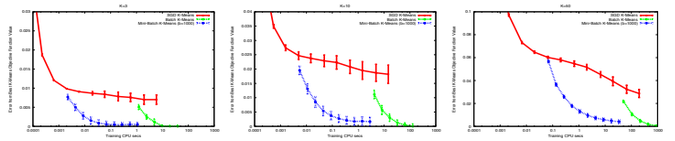

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  $M \leftarrow b$ examples picked randomly from X
  for $\mathbf{x} \in M$ **do**
    $\mathbf{d}[\mathbf{x}] \leftarrow f(C, \mathbf{x})$ // Cache the center nearest to $\mathbf{x}$
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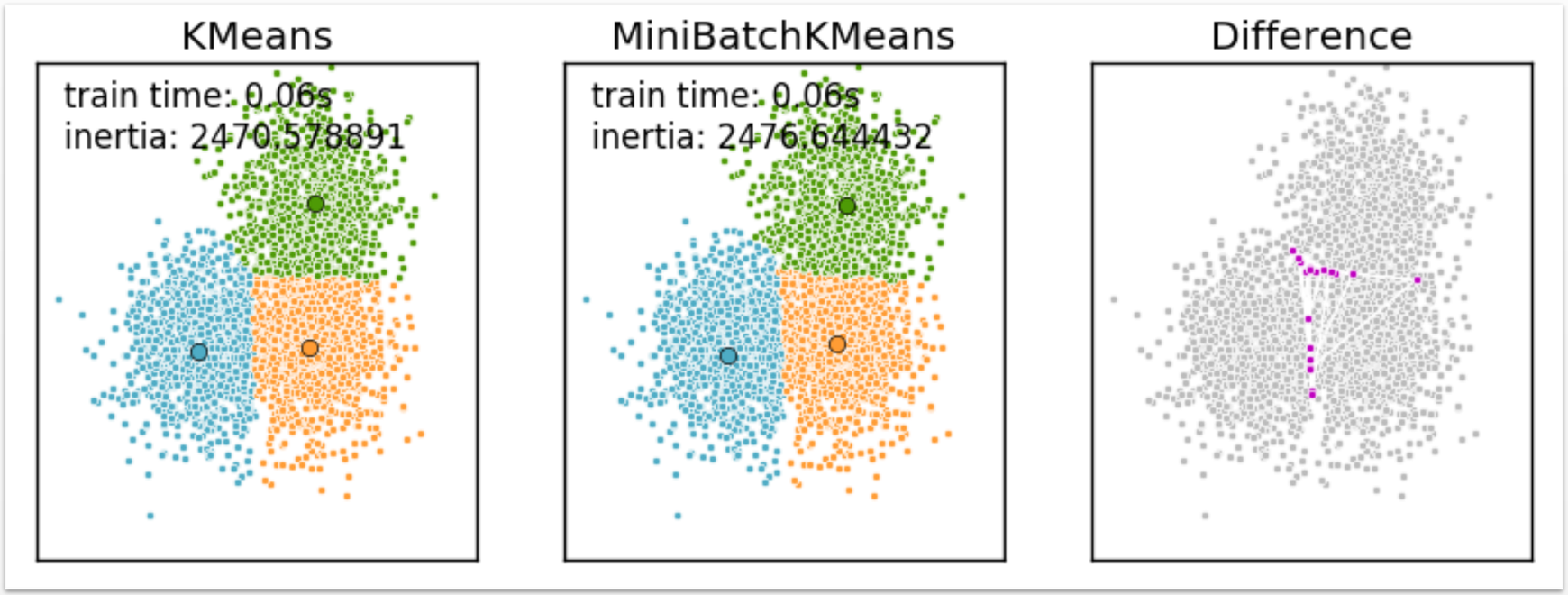
  end for
end for

Complexity: O(~~N~~ M K D t)

Here t is the number of iterations

Mini-batch K-means



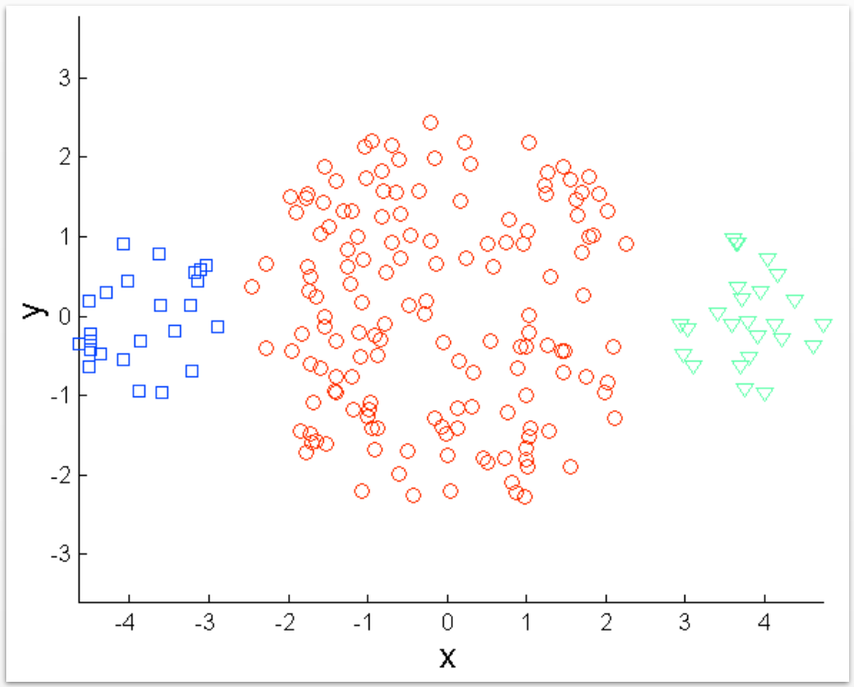
Clustering

Shantanu Jain

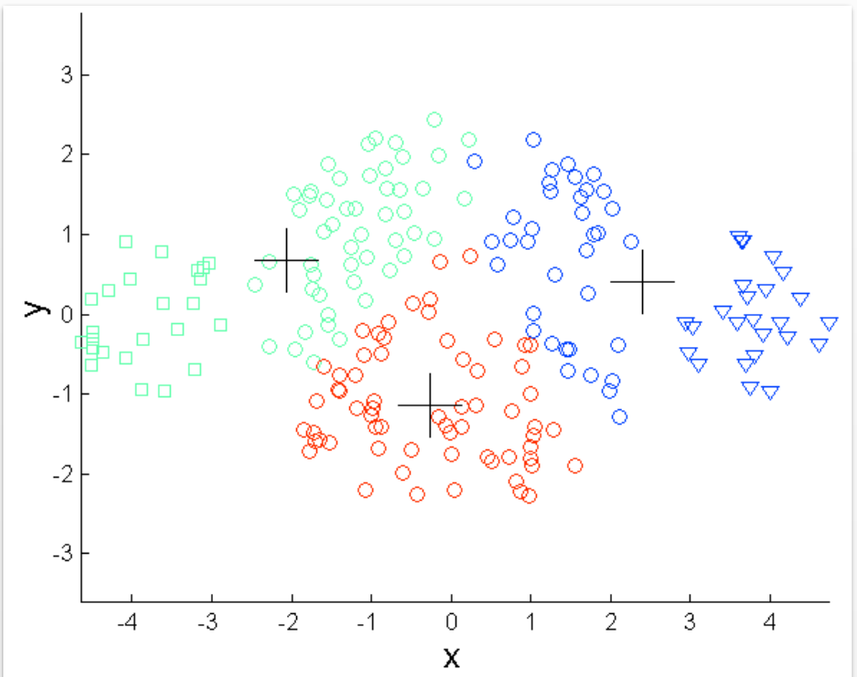
K-means Clustering

Limitations

K-means Limitations: Differing Sizes

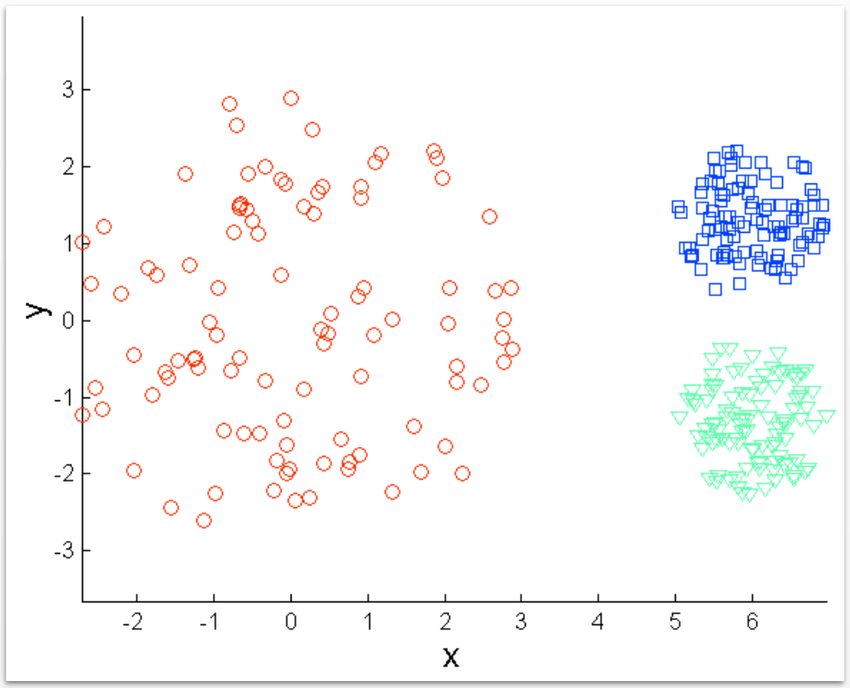


Original Points

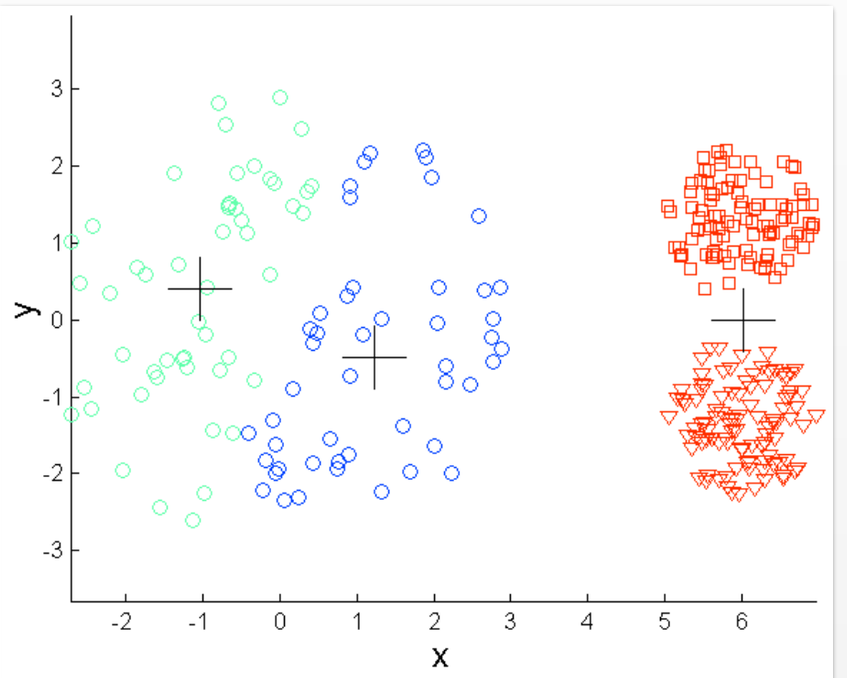


K-means (3 clusters)

K-means Limitations: Different Densities

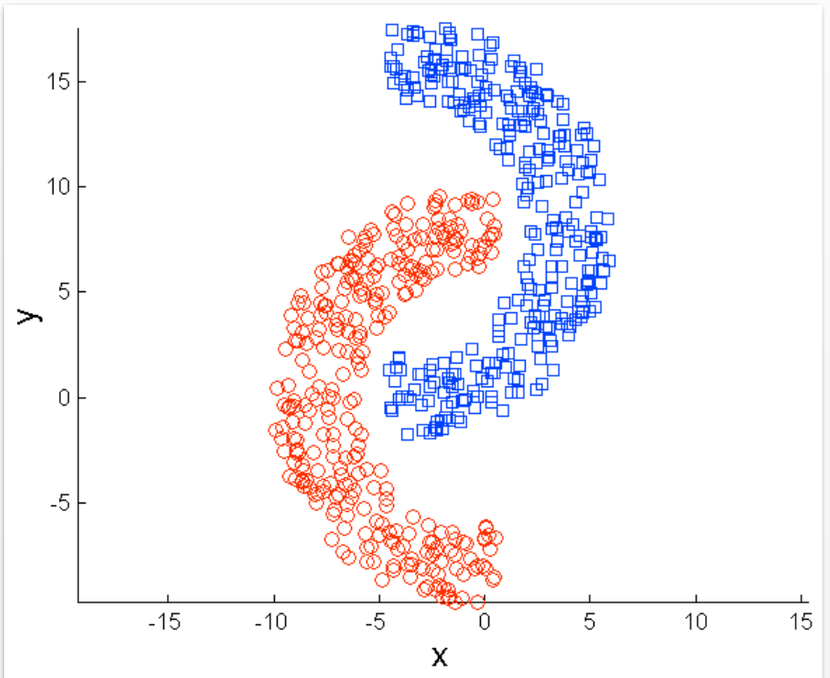


Original Points

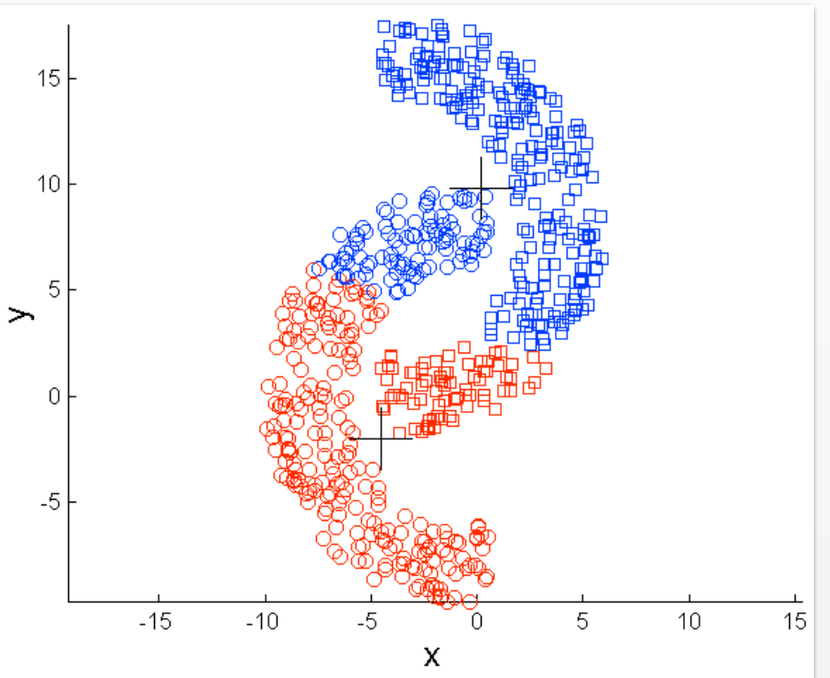


K-means (3 clusters)

K-means Limitations: Non-globular Shapes

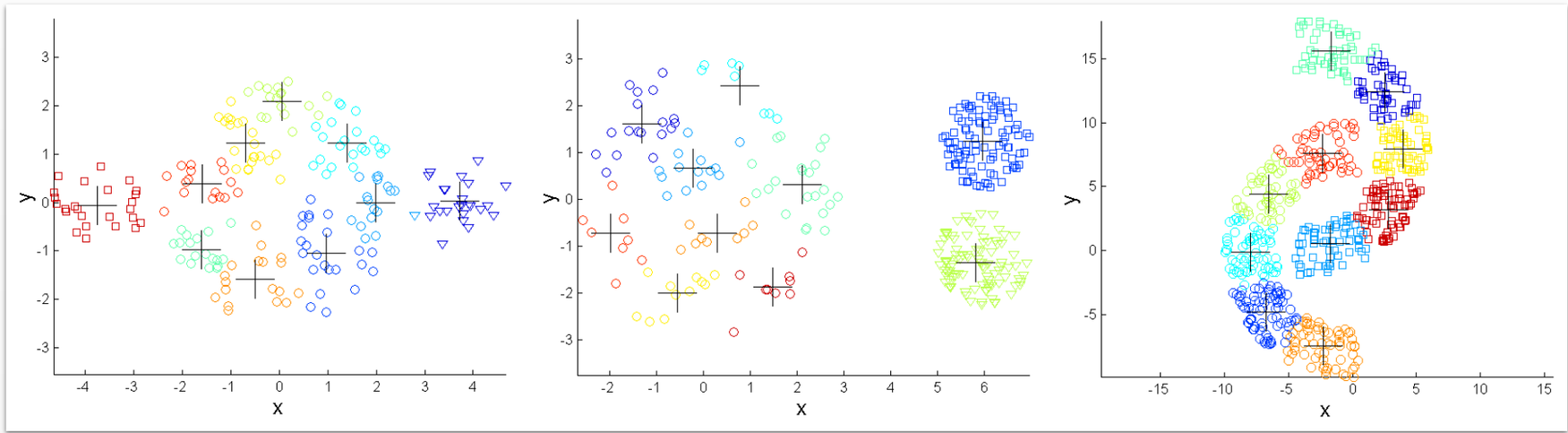


Original Points



K-means (2 clusters)

Overcoming K-means Limitations



Intuition: “Combine” smaller clusters into larger clusters

- *One Solution:* Hierarchical Clustering
- *Another Solution:* Density-based Clustering