New Developments In The Theory Of Clustering

that’s all very well in practice, but does it work in theory?

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Overview

What we will cover

A few of the recent theory results on clustering:

- Practical algorithms that have strong theoretical guarantees
- Models to explain behavior observed in practice
What we will not cover

The rest:

- Recent strands of theory of clustering such as metaclustering and privacy preserving clustering
- Clustering with distributional data assumptions
- Proofs
Outline

I Euclidean Clustering and k-means algorithm

II Bregman Clustering and k-means

III Stability
Outline

I Euclidean Clustering and $k$-means algorithm
  - What to do to select initial centers (and what not to do)
  - How long does $k$-means take to run in theory, practice and theoretical practice
  - How to run $k$-means on large datasets

II Bregman Clustering and $k$-means

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II Bregman Clustering and $k$-means
- Bregman Clustering as generalization of $k$-means
- Performance Results

III Stability
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I Euclidean Clustering and \texttt{k-means} algorithm

- What to do to select initial centers (and what not to do)
- How long does \texttt{k-means} take to run in theory, practice and theoretical practice
- How to run \texttt{k-means} on large datasets

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- Bregman Clustering as generalization of \texttt{k-means}
- Performance Results

III Stability

- How to relate closeness in cost function to closeness in clusters.
Euclidean Clustering and \( k \)-means
What does it mean to cluster?

Given $n$ points in $\mathbb{R}^d$ find the best way to split them into $k$ groups.
Introduction

How do we define “best”?

Example:
Introduction

How do we define “best”?

Example:

Clustering

Given $n$ points in $\mathbb{R}^d$ split them into $k$ similar groups.
How do we define “best”? Minimize the maximum radius of a cluster.
Introduction

How do we define “best”? 
Maximize the average inter-cluster distance
How do we define “best”? Minimize the variance within each cluster.
Introduction

How do we define “best”? Minimize the variance within each cluster.

Minimizing total variance

For each cluster $C_i \in \mathcal{C}$, $c_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$ is the expected location of a point in a cluster.

Then the variance of each cluster is:

$$\sum_{x \in C_i} = \|x - c_i\|^2$$

And the total objective is:

$$\phi = \sum_{C_i} \sum_{x \in C_i} \|x - c_i\|^2$$

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Approximations

Minimizing Variance

Given $X$ and $k$, find a clustering $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ that minimizes:

$$\phi(X, \mathcal{C}) = \sum_{c_i} \sum_{x \in C_i} \|x - c_i\|^2$$
Approximations

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Definition

Let $\phi^*$ denote the value of the optimum solution above. We say that a clustering $\mathcal{C}'$ is $\alpha$-approximate if:

$$\phi^* \leq \phi(X, \mathcal{C}') \leq \alpha \cdot \phi^*$$
Approximations

Minimizing Variance

Given $X$ and $k$, find a clustering $C = \{C_1, C_2, \ldots, C_k\}$ that minimizes:

$$\phi(X, C) = \sum_{c_i} \sum_{x \in C_i} \|x - c_i\|^2$$

Solving this problem

This problem is NP-complete, even when the pointset $X$ lies in two dimensions...
Minimizing Variance

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Solving this problem

This problem is NP-complete, even when the pointset $X$ lies in two dimensions...

...but we’ve been solving it for over 50 years! [S56][L57][M67]
k-means

Example

Given a set of data points

Lloyd's Method: k-means
Initialize with random clusters

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Example

Given a set of data points
Example

Select initial centers at random
Example

Assign each point to nearest center
k-means

Example

Recompute optimum centers given a fixed clustering
k-means

Example
Repeat

Lloyd's Method: k-means
Repeat: Assign points to nearest center
Example
Repeat

Lloyd's Method: k-means
Repeat: Recompute centers
20
k-means

Example
Repeat
Example

Until the clustering doesn’t change
This algorithm terminates!

Recall the total error:

$$\phi(X, \mathcal{C}) = \sum_{i} \sum_{x \in C_i} ||x - c_i||^2$$

In every iteration $\phi$ is reduced:

- Assigning each point to the nearest center reduces $\phi$
- Given a fixed cluster, the mean is the optimal location for the center (requires proof)
The algorithm finds a local minimum …
Performance

... that’s potentially arbitrarily worse than optimum solution
But does this really happen?
But does this really happen? YES!
Performance

Finding a good set of initial points is a black art
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- Try many times with different random seeds
  - Most common method
  - Has limited benefit even in case of Gaussians
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  - Hundreds of heuristics
  - Including pre & post processing ideas
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There exists a fast and simple initialization scheme with provable performance guarantees
Random Initializations on Gaussians

Some Gaussians are combined
But the Gaussian case has an easy fix: use a furthest point heuristic.
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Seeding on Gaussians

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Seeding on Gaussians

But this fix is overly sensitive to outliers
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But this fix is overly sensitive to outliers.
What if we interpolate between the two methods?

Let $D(x)$ be the distance between a point $x$ and its nearest cluster center. Choose the next point proportionally to $D^\alpha(x)$.

- $\alpha = 0 \Rightarrow$ Random initialization
- $\alpha = \infty \Rightarrow$ Furthest point heuristic
- $\alpha = 2 \Rightarrow k$-means++

More generally, set the probability of selecting a point proportional to its contribution to the overall error.

- If minimizing $\sum c_i \sum_{x \in C_i} \|x - c_i\|$, sample according to $D$.
- If minimizing $\sum c_i \sum_{c_i \in C_i} \|x - c_i\|_\infty$, sample according to $D_\infty$ (take the furthest point).
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k-means++

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More generally

Set the probability of selecting a point proportional to its contribution to the overall error.

- If minimizing $\sum_{c_i} \sum_{x \in C_i} ||x - c_i||$, sample according to $D$.
- If minimizing $\sum_{c_i} \sum_{c \in C_i} ||x - c_i||_\infty$, sample according to $D^\infty$ (take the furthest point).
Example of $k$-means++

If the data set looks Gaussian...
Example of k-means++

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If the data set looks Gaussian...
Example of k-means++

If the outlier should be its own cluster . . .
Example of \textit{k-means++}

If the outlier should be its own cluster \ldots
Example of k-means++

If the outlier should be its own cluster ...
Example of $k$-means++

If the outlier should be its own cluster ...
Example of k-means++

If the outlier should be its own cluster ...
What can we say about performance of k-means++?

Theorem (AV07)
This algorithm always attains an $O(\log k)$ approximation in expectation.

Theorem (ORSS06)
A slightly modified version of this algorithm attains an $O(1)$ approximation if the data is ‘nicely clusterable’ with $k$ clusters.
Analyzing $k$-means++

What can we say about performance of $k$-means++?

**Theorem (AV07)**

*This algorithm always attains an $O(\log k)$ approximation in expectation.*
What can we say about performance of k-means++?

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A slightly modified version of this algorithm attains an $O(1)$ approximation if the data is ‘nicely clusterable’ with $k$ clusters.
What do we mean by ‘nicely clusterable’?

Intuitively, $X$ is nicely clusterable if going from $k-1$ to $k$ clusters drops the total error by a constant factor.
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Intuitively, $X$ is nicely clusterable if going from $k - 1$ to $k$ clusters drops the total error by a constant factor.

**Definition**

A pointset $X$ is $(k, \varepsilon)$-separated if $\phi_k^*(X) \leq \varepsilon^2 \phi_{k-1}^*(X)$. 
Why does this work?

**Intuition**

Look at the optimum clustering. In expectation:

1. If the algorithm selects a point from a new OPT cluster, that cluster is covered pretty well
2. If the algorithm picks two points from the same OPT cluster, then other clusters must contribute little to the overall error
Why does this work?

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Look at the optimum clustering. In expectation:

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As long as the points are reasonably well separated, the first condition holds.
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**Intuition**

Look at the optimum clustering. In expectation:

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2. If the algorithm picks two points from the same OPT cluster, then other clusters must contribute little to the overall error.

As long as the points are reasonably well separated, the first condition holds.

**Two theorems**

- Assume the points are \((k, \varepsilon)\)-separated and get an \(O(1)\) approximation.
- Make no assumptions about separability and get an \(O(\log k)\) approximation.
k-means++ Summary:

- To select the next cluster, sample a point in proportion to its current contribution to the error.
- Works for $k$-means, $k$-median, other objective functions.
- Universal $O(\log k)$ approximation, $O(1)$ approximation under some assumptions.
- Can be implemented to run in $O(nkd)$ time (same as a single $k$-means step).
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But does it actually work?
Large Evaluation

<table>
<thead>
<tr>
<th>Data set</th>
<th>$\phi: k$-means++ vs $k$-means $(k = 10, 25, 50, 100)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.011 1.036 1.115 1.544</td>
</tr>
<tr>
<td>2</td>
<td>1.052 1.344 1.523 1.421</td>
</tr>
<tr>
<td>3</td>
<td>1.122 2.083 2.987 3.481</td>
</tr>
<tr>
<td>4</td>
<td>1.007 1.206 1.207 1.421</td>
</tr>
<tr>
<td>5</td>
<td>1.038 1.303 1.367 1.861</td>
</tr>
<tr>
<td>6</td>
<td>1.010 1.013 1.018 1.043</td>
</tr>
<tr>
<td>7</td>
<td>1.027 1.160 1.560 2.056</td>
</tr>
<tr>
<td>8</td>
<td>0.997 1.009 1.044 1.186</td>
</tr>
<tr>
<td>9</td>
<td>1.090 1.181 1.314 1.297</td>
</tr>
<tr>
<td>10</td>
<td>13.87 132.7 684.9 3728</td>
</tr>
<tr>
<td>11</td>
<td>1.002 1.003 1.011 1.046</td>
</tr>
<tr>
<td>12</td>
<td>2.420 5.027 11.08 22.76</td>
</tr>
<tr>
<td>13</td>
<td>2.202 9.532 11.96 30.17</td>
</tr>
<tr>
<td>14</td>
<td>1.020 1.039 7.942 1.008</td>
</tr>
<tr>
<td>15</td>
<td>1.013 554.2 1.003 1.004</td>
</tr>
<tr>
<td>Range</td>
<td>[0.997, 3728]</td>
</tr>
<tr>
<td>Median</td>
<td>1.207</td>
</tr>
<tr>
<td>Mean</td>
<td>87.93</td>
</tr>
</tbody>
</table>
Typical Run

KM++ v. KM v. KM-Hybrid

Stage vs. Error for LLOYD, HYBRID, and KM++ methods.
Other Runs

KM++ v. KM v. KM-Hybrid

Error vs. Stage

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How fast does k-means converge?

It appears the algorithm converges in under 100 iterations (even faster with smart initialization).
How fast does $k$-means converge?

It appears the algorithm converges in under 100 iterations (even faster with smart initialization).

Theorem (V09)

There exists a pointset $X$ in $\mathbb{R}^2$ and a set of initial centers $\mathcal{C}$ so that $k$-means takes $2^{\Omega(k)}$ iterations to converge when initialized with $\mathcal{C}$. 

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Finding the disconnect

In theory:
  - \textit{k-means} might run in exponential time

In practice:
  - \textit{k-means} converges after a handful of iterations

It works in practice but it does not work in theory!
Finding the disconnect

Robustness of worst case examples
Perhaps the worst case examples are too precise, and can never arise out of natural data

Quantifying the robustness
If we slightly perturb the points of the example:
• The optimum solution shouldn’t change too much
• Will the running time stay exponential?
Small Perturbations

Huge gap between worst-case and observed results. Check how fragile the worst case is. Add a little bit of noise to the data before running the algorithm.
Small Perturbations

Huge gap between worst-case and observed results. Check how fragile the worst case is. Add a little bit of noise to the data before running the algorithm. Optimum solution barely changes.
Small Perturbations

Huge gap between worst-case and observed results. Check how fragile the worst case is. Add a little bit of noise to the data before running the algorithm.
Smoothed Analysis

**Perturbation**

To each point $x \in X$ add independent noise drawn from $N(0, \sigma^2)$.

**Definition**

The smoothed complexity of an algorithm is the maximum expected running time after adding the noise:

$$\max_X \mathbb{E}_\sigma [Time(X + \sigma)]$$
Smoothed Analysis

Theorem (AMR09)

The smoothed complexity of \textit{k-means} is bounded by

\[ O\left(\frac{n^{34}k^{34}d^8D^6 \log^4 n}{\sigma^6}\right) \]

Notes

- While the bound is large, it is not exponential ($2^k \gg k^{34}$ for large enough $k$)
- The ($D/\sigma)^6$ factor shows the bound is scale invariant
Comparing bounds

The smoothed complexity of $k$-means is polynomial in $n, k$ and $D/\sigma$ where $D$ is the diameter of $X$, whereas the worst case complexity of $k$-means is exponential in $k$.

Implications

The pathological examples:

- Are very brittle
- Can be avoided with a little bit of random noise
## k-means Summary

### Running Time
- Exponential worst case running time
- Polynomial typical case running time
**k-means Summary**

**Running Time**
- Exponential worst case running time
- Polynomial typical case running time

**Solution Quality**
- Arbitrary local optimum, even with many random restarts
- Simple initialization leads to a good solution
Implementing \texttt{k-means++}

Initialization:
- Takes $O(nd)$ time and one pass over the data to select the next center
- Takes $O(nkd)$ time total

Overall running time:
- Each round of \texttt{k-means} takes $O(nkd)$ running time
- Typically finish after a constant number of rounds
Implementing $k$-means++

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Large Data

What if $O(nkd)$ is too much, can we parallelize this algorithm?
Parallelizing k-means

**Approach**

Partition the data:

- Split $X$ into $X_1, X_2, \ldots, X_m$ of roughly equal size.
Parallelizing $k$-means

Approach

Partition the data:

- Split $X$ into $X_1, X_2, \ldots, X_m$ of roughly equal size.

In parallel compute a clustering on each partition:

- Find $\mathcal{C}^j = \{C_1^j, \ldots, C_k^j\}$: a good clustering on each partition, and denote by $w_i^j$ the number of points in cluster $C_i^j$. 

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Parallelizing k-means

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In parallel compute a clustering on each partition:

- Find $C_j = \{C^j_1, \ldots, C^j_k\}$: a good clustering on each partition, and denote by $w^j_i$ the number of points in cluster $C^j_i$.

Cluster the clusters:

- Let $Y = \bigcup_{1 \leq j \leq m} C^j$. Find a clustering of $Y$, weighted by the weights $W = \{w^j_i\}$. 

Parallelization Example

Given $X$
Parallelization Example

Partition the dataset
Parallelization Example

Cluster each partition separately
Parallelization Example

Cluster each partition separately
Parallelization Example

Cluster each partition separately
Parallelization Example

Cluster each partition separately
Parallelization Example

Cluster the clusters
Parallelization Example

Cluster the clusters
Parallelization Example

Cluster the clusters
Parallelization Example

Final clustering:
Parallelization Example

Final clustering:
Quality of the solution

What happens when we approximate the approximation?

- Suppose the algorithm in phase 1 gave a $\beta$-approximate solution to its input
- Algorithm in phase 2 gave a $\gamma$-approximate solution to its (smaller) input
Quality of the solution

What happens when we approximate the approximation?

- Suppose the algorithm in phase 1 gave a $\beta$-approximate solution to its input

- Algorithm in phase 2 gave a $\gamma$-approximate solution to its (smaller) input

Theorem (GNMO00, AJM09)

*The two phase algorithm gives a $4\gamma(1 + \beta) + 2\beta$ approximate solution.*
Running time

Suppose we partition the input across $m$ different machines.

- First phase running time: $O\left(\frac{nk^d}{m}\right)$.
- Second phase running time $O(mk^2d)$. 
Improving the algorithm

Approximation Guarantees

Using \texttt{k-means++} sets $\beta = \gamma = O(\log k)$ and leads to a $O(\log^2 k)$ approximation.
Improving the algorithm

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Using $k$-means++ sets $\beta = \gamma = O(\log k)$ and leads to a $O(\log^2 k)$ approximation.

Improving the Approximation
Must improve the approximation guarantee of the first round, but can use a larger $k$ to ensure every cluster is well summarized.
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Improving the Approximation
Must improve the approximation guarantee of the first round, but can use a larger $k$ to ensure every cluster is well summarized.

Theorem (ADK09)
Running $k$-means++ initialization for $O(k)$ rounds leads to a $O(1)$ approximation to the optimal solution (but uses more centers than OPT).
Final Algorithm

Partition the data:

- Split $X$ into $X_1, X_2, \ldots, X_m$ of roughly equal size.
Final Algorithm

Partition the data:

- Split $X$ into $X_1, X_2, \ldots, X_m$ of roughly equal size.

Compute a clustering using $\ell = O(k)$ centers each partition:

- Find $\mathcal{C}^j = \{C_1^j, \ldots, C_\ell^j\}$ using $k$-means++ on each partition, and denote by $w_i^j$ the number of points in cluster $C_i^j$. 

Cluster the clusters.

Let $Y = \bigcup_{1 \leq j \leq m} C_j$ be a set of $O(\ell m)$ points. Use $k$-means++ to cluster $Y$, weighted by the weights $W = \{w_i^j\}$.
Two round \texttt{k-means++}

**Final Algorithm**

Partition the data:

- Split $X$ into $X_1, X_2, \ldots, X_m$ of roughly equal size.

Compute a clustering using $\ell = O(k)$ centers each partition:

- Find $\mathcal{C}^j = \{C^j_1, \ldots, C^j_\ell\}$ using \texttt{k-means++} on each partition, and denote by $w^j_i$ the number of points in cluster $C^j_i$.

Cluster the clusters.

- Let $Y = \bigcup_{1 \leq j \leq m} \mathcal{C}^j$ be a set of $O(\ell m)$ points. Use \texttt{k-means++} to cluster $Y$, weighted by the weights $W = \{w^j_i\}$.

**Theorem**

The algorithm achieves an $O(1)$ approximation in time $O\left(\frac{nk^d}{m} + mk^2d\right)$
Summary

Before...
k-means used to be a prime example of the disconnect between theory and practice – it works well, but has horrible worst case analysis

...and after
Smoothed analysis explains the running time and rigorously analyzed initializations routines help improve clustering quality.
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- How to relate closeness in cost function to closeness in clusters.
Clustering With Non-Euclidean Metrics
Application I: Clustering Documents

Kullback-Leibler distance:

\[ D(p, q) = \sum_i p_i \log \frac{p_i}{q_i} \]
Kullback-Leibler distance:

\[ D(p, q) = \sum_i p_i \log \frac{p_i}{q_i} \]
Application III: Speech Analysis

Itakuro-Saito distance:

\[ D(p, q) = \sum_i \frac{p_i}{q_i} - \log \frac{p_i}{q_i} - 1 \]
Bregman Divergences

Definition

Let $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ be a strictly convex function. The Bregman divergence $d_\phi$ is defined as

$$D_\phi(x \parallel y) = \phi(x) - \phi(y) - \langle \nabla \phi(y), x - y \rangle$$

Examples:

Kullback-Leibler: $\phi(x) = \sum x_i \ln x_i - x_i$, $D_\phi(x \parallel y) = \sum x_i \ln \frac{x_i}{y_i}$

Itakura-Saito: $\phi(x) = -\sum \ln x_i$, $D_\phi(x \parallel y) = \sum_i \frac{x_i}{y_i} - \log \frac{x_i}{y_i} - 1$

$\ell_2^2$: $\phi(x) = \frac{1}{2}||x||^2$, $D_\phi(x \parallel y) = ||x - y||^2$
Overview

$k$-means clustering $\equiv$ Bregman clustering

- The algorithm works the same way.
- Same (bad) worst-case behavior
- Same (good) smoothed behavior
- Same (good) quality guarantees, with correct initialization
Properties

\[ D_\phi(x \parallel y) = \phi(x) - \phi(y) - \langle \nabla \phi(y), x - y \rangle \]

- Asymmetry: In general, \( D_\phi(p \parallel q) \neq D_\phi(q \parallel p) \)
- No triangle inequality: \( D_\phi(p \parallel q) + D_\phi(q \parallel r) \) can be less than \( D_\phi(p \parallel r) \)!

How can we now do clustering?

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Breaking down $k$-means

Initialize cluster centers
while not converged do
    Assign points to nearest cluster center
    Find new cluster center by averaging points assigned together
end while

Key Point
Setting cluster center as centroid minimizes the average **squared distance** to center
Breaking down \textit{k}-means

Initialize cluster centers
\textbf{while} not converged \textbf{do}
  Assign points to nearest cluster center
  \par FIND new cluster center by averaging points assigned together
\textbf{end while}

\textbf{Key Point}

Setting cluster center as centroid minimizes the average \textit{squared} distance to center
Problem

Given points $x_1, \ldots, x_n \in \mathbb{R}^d$, find $c$ such that

$$\sum_i D_\phi(x_i \| c)$$

is minimized.

Answer

$$c = \frac{1}{n} \sum x_i$$

Independent of $\phi$ [BMDG05]!
Bregman $k$-means

Initialize cluster centers

while not converged do
    Assign points to nearest cluster center (by measuring $D_{\phi}(x \parallel c)$)
    Find new cluster center by averaging points assigned together
end while

Key Point
Setting cluster center as centroid minimizes average Bregman divergence to center
Lemma ([BMDG05])

The (Bregman) k-means algorithm converges in cost.

Euclidean distance:
The quantity

$$\sum_{C} \sum_{x \in C} \|x - \text{center}(C)\|^2$$

decreases with each iteration of $k$-means

Bregman divergence: Bregman Information:

$$\sum_{C} \sum_{x \in C} D_\phi(x \| \text{center}(C))$$

decreases with each iteration of the Bregman $k$-means algorithm.
EM and Soft Clustering

Expectation maximization:

Initialize density parameters and means for $k$ distributions

while not converged do

For distribution $i$ and point $x$, compute conditional probability $p(i|x)$ that $x$ was drawn from $i$ (by Bayes rule)

For each distribution $i$, recompute new density parameters and means (via maximum likelihood)

end while

This yields a soft clustering of points to “clusters”

Originally used for mixtures of Gaussians.
Definition (Exponential Family)

Parametric family of distributions $p_{\Psi, \theta}$ is an exponential family if each density is of the form

$$p_{\Psi, \theta} = \exp(\langle x, \theta \rangle - \Psi(\theta))p_0(x)$$

with $\Psi$ convex.

Let $\phi(t) = \Psi^*(t)$ be the Legendre-Fenchel dual of $\Psi(x)$:

$$\phi(t) = \sup_x (\langle x, t \rangle - \Psi(x))$$

Theorem ([BMDG05])

$$p_{\Psi, \theta} = \exp(-D_\phi(x \| \mu))b_\phi(x)$$

where $\mu$ is the expectation parameter $\nabla \Psi(\theta)$
Expectation maximization:
Initialize density parameters and means for $k$ distributions

while not converged do
    For distribution $i$ and point $x$, compute conditional probability $p(i|x)$ that $x$ was drawn from $i$ (by Bayes rule)
    For each distribution $i$, recomputee new density parameters and means (via maximum likelihood)
end while

Choosing the corresponding Bregman divergence $D_\phi(\cdot \mid \cdot)$, $\phi = \Psi^*$ gives mixture density estimation for any exponential family $p_{\Psi,\theta}$.
Performance Analysis
Performance Analysis

Two questions:

Problem (Rate of convergence)

Given an arbitrary set of $n$ points in $d$ dimensions, how long does it take for (Bregman) $k$-means to converge?

Problem (Quality of Solution)

Let $\text{OPT}$ denote the optimal clustering that minimizes the average sum of (Bregman) distances to cluster centers. How close to $\text{OPT}$ is the solution returned by (Bregman) $k$-means?
Two questions:

**Problem (Rate of convergence)**

Given an arbitrary set of $n$ points in $d$ dimensions, how long does it take for (Bregman) k-means to converge?

**Problem (Quality of Solution)**

Let $OPT$ denote the optimal clustering that minimizes the average sum of (Bregman) distances to cluster centers. How close to $OPT$ is the solution returned by (Bregman) k-means?
Performance Analysis

Two questions:

Problem (Rate of convergence)

*Given an arbitrary set of n points in d dimensions, how long does it take for (Bregman) k-means to converge?*
Convergence of \( k \)-means

Parameters: \( n, k, d \).

😊 Good news

\( k \)-means always converges in \( O(n^{kd}) \) time.

😢 Bad news

\( k \)-means can take time \( 2^{\Omega(k)} \) to converge:
Convergence of $k$-means

Parameters: $n, k, d$.

😊 Good news

$k$-means always converges in $O(n^{kd})$ time.

😢 Bad news

$k$-means can take time $2^{\Omega(k)}$ to converge:
- Even if $d = 2$, i.e., in the plane
Convergence of $k$-means

Parameters: $n, k, d$.

😊 Good news
$k$-means always converges in $O(n^{kd})$ time.

😊 Bad news
$k$-means can take time $2^\Omega(k)$ to converge:
- Even if $d = 2$, i.e. in the plane
- Even if centers are chosen from the initial data
Convergence of Bregman $k$-means

Euclidean distance:
k-means can take time $2^{\Omega(k)}$ to converge:
- Even if $d = 2$, i.e. in the plane
- Even if centers are chosen from the initial data

Bregman divergence:
For some Bregman divergences, $k$-means can take time $2^{\Omega(k)}$ to converge [MR09]:
- Even if $d = 2$, i.e. in the plane
- Even if centers are chosen from the initial data
Proof Idea

"Well behaved" Bregman divergences look "locally Euclidean":

\[ \{ x \mid \|x - c\|^2 \leq 1 \} \quad \text{and} \quad \{ x \mid D_\phi(x, c) \leq 1 \} \]

Take a bad Euclidean instance and shrink it to make it local.
Smoothed Analysis

Real inputs aren’t worst-case!

Analyze expected run-time over perturbations.
Smoothed Analysis

Real inputs aren’t worst-case!

Analyze *expected* run-time over perturbations.
**Theorem**

*Smoothed complexity of k-means using Gaussian noise with variance $\sigma$ is *polynomial* in $n$ and $1/\sigma$.*

Compare this to worst-case lower bound of $2^{\Theta(n)}$.
Normal smoothing doesn’t work!

\[ \Delta_n = \{(x_1, \ldots, x_n) \mid \sum x_i = 1\} \]
More general notion of smoothing:
More general notion of smoothing:

- perturbation should stay close to a hyperplane
Bregman smoothing

More general notion of smoothing:

- perturbation should stay close to a hyperplane
- density of perturbation is proportional to $1/\sigma^d$
Bregman smoothing: Results

Theorem ([MR09])

For “well-behaved” Bregman divergences, smoothed complexity is bounded by $\text{poly}(n^{\sqrt{k}}, 1/\sigma)$ and $k^{kd}\text{poly}(n, 1/\sigma)$.

This is in comparison to worst-case bound of $2^{\Omega(n)}$. 
Performance Analysis

Two questions:

Problem (Rate of convergence)
Given an arbitrary set of \( n \) points in \( d \) dimensions, how long does it take for (Bregman) \( k \)-means to converge?

Problem (Quality of Solution)
Let \( OPT \) denote the optimal clustering that minimizes the average sum of (Bregman) distances to cluster centers. How close to \( OPT \) is the solution returned by (Bregman) \( k \)-means?
Performance Analysis

Two questions:

Problem (Quality of Solution)

Let $OPT$ denote the optimal clustering that minimizes the average sum of (Bregman) distances to cluster centers. How close to $OPT$ is the solution returned by (Bregman) $k$-means?
Problem

Given $x_1, \ldots, x_n$, and parameter $k$, find $k$ centers $c_1, \ldots, c_k$ such that

$$\sum_{x=1}^{n} \min_{j=1}^{k} d(x_i, c_j)$$

is minimized.
Problem

Given \( x_1, \ldots, x_n \), and parameter \( k \), find \( k \) centers \( c_1, \ldots, c_k \) such that

\[
\sum_{x=1}^{n} \min_{j=1}^{k} d(x_i, c_j)
\]

is minimized.

Problem (c-approximation)

Let \( \text{OPT} \) be the optimal solution above. Fix \( c > 0 \). Find centers \( c'_1, \ldots, c'_k \) such that if

\[
A = \sum_{x=1}^{n} \min_{j=1}^{k} d(x_i, c'_j)
\]

then

\[
\text{OPT} \leq A \leq c \cdot \text{OPT}
\]
Initialization

- Let distance from \( x \) to nearest cluster center be \( D(x) \)
- Pick \( x \) as new center with probability

\[
p(x) \propto D^2(x)
\]

Properties of solution:

- For arbitrary data, this gives \( O(\log n) \)-approximation
- For “well-separated data”, this gives constant \( (O(1)) \)-approximation.
Informally, data is \((k, \alpha)\)-well separated if the best clustering that uses \(k - 1\) clusters has cost that is \(\geq 1/\alpha \cdot \text{OPT}\).
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Bregman $k$-means++

**Initialization**
- Let Bregman divergence from $x$ to nearest cluster center be $D(x)$
- Pick $x$ as new center with probability
  
  $$p(x) \propto D(x)$$

Run algorithm as before.

**Theorem ([AB09, AB10])**
- $O(1)$-approximation for $(k, \alpha)$-separated sets.
- $O(\log n)$ approximation in general.
Stability in clustering
Two measures of cost:

- Distance between clusterings \( \mathcal{C}, \mathcal{C}^* \):
  \[
d(\mathcal{C}, \mathcal{C}^*) = \text{fraction of points on which they disagree}
\]

- (Quality) distance from \( \mathcal{C} \) to OPT:
  \[
d_q(\mathcal{C}, \text{OPT}) = \frac{\text{cost}(\mathcal{C})}{\text{cost}(\text{OPT})}
\]

Can closeness in \( d_q \) imply closeness in \( d \)?
NP-hardness

NP-hardness is an obstacle to finding good clusterings.

- $k$-means and $k$-median are NP-hard, and hard to approximate in general graphs
- $k$-means, $k$-median can be approximated in $\mathbb{R}^d$ but seem to need time exponential in $d$
- Same is true for Bregman clustering [CM08]
What happens if target clustering and optimal clustering are not the same?

The two distance functions might be incompatible.
Target And Optimal Clusterings

What happens if target clustering and optimal clustering are not the same?

The two distance functions might be incompatible.
Stability Of Clusterings

An instance is *stable* if approximating the cost function gives us a solution close to the target clustering.

**View 1:** If we perturb inputs, the output should not change.
An instance is *stable* if approximating the cost function gives us a solution close to the target clustering.

**View 1:** If we perturb inputs, the output should not change.

**View 2:** If we change the distance function, output should not change.
Stability Of Clusterings

An instance is *stable* if approximating the cost function gives us a solution close to the target clustering.

**View 1:** If we perturb inputs, the output should not change.

**View 2:** If we change the distance function, output should not change.

**View 3:** If we change the cost quality of solution, then output should not change.
Stability I: Perturbing Inputs

Well separated sets:

Data is \((k, \alpha)\)-well separated if the best clustering that uses \(k - 1\) clusters has cost that is \(\geq 1/\alpha \cdot \text{OPT}\).

Two interesting properties[ORSS06]:
- All optimal clusterings mostly look the same: \(d_q\) small \(\Rightarrow d\) small.
- Small perturbations of the data don’t change this property.

Computationally, well-separatedness makes \(k\)-means work well
Stability II: Perturbing Distance Function

**Definition (α-perturbations[BL09])**

A clustering instance \((P,d)\) is \(\alpha\)-perturbation-resilient if the optimal clustering is identical to the optimal clustering for any \((P,d')\), where

\[
d(x,y)/\alpha \leq d'(x,y) \leq d(x,y) \cdot \alpha
\]

- The smaller the \(\alpha\), the more resilient the instance (and the more “stable”)
- Center-based clustering problems (\(k\)-median, \(k\)-means, \(k\)-center) can be solved optimally for \(\sqrt{3}\)-perturbation-resilient inputs[ABS10]

Sergei V. and Suresh V. Theory of Clustering
Definition \(((c, \varepsilon)\text{-property}[\text{BBG09}])\)

Given an input, all clusterings that are \(c\)-approximate are also \(\varepsilon\)-close.

Surprising facts:

- Finding a \(c\)-approximation in general might be NP-hard.
- Finding a \(c\)-approximation here is easy!
Proof Idea

- If near-optimal clusters are close to true answer, then clusters must be well-separated.
- If clusters are well-separated, then choosing the right threshold separates them cleanly.
- Important that **ALL** near-optimal clusterings are close to true answer.
Proof Idea

- If near-optimal clusters are close to true answer, then clusters must be well-separated.
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Proof Idea

- If near-optimal clusters are close to true answer, then clusters must be well-separated.
- If clusters are well-separated, then choosing the right threshold separates them cleanly.
- Important that **ALL** near-optimal clusterings are close to true answer.
Main Result

**Theorem**

In polynomial time, we can find a clustering that is $O(\epsilon)$-close to the target clustering, even if finding a $c$-approximation is NP-hard.
Generalization

Strong assumption: **ALL** near-optimal clusterings are close to true answer.

Variant [ABS10]: Only consider *Voronoi*-based clusterings, where each point is assigned to *nearest* cluster center.

Same results hold as for previous case.
Generalization

Strong assumption: **ALL** near-optimal clusterings are close to true answer.

Variant[ABS10]: Only consider *Voronoi*-based clusterings, where each point is assigned to *nearest* cluster center.

Same results hold as for previous case.
Wrap Up
We understand much more about the behavior of $k$-means, and why it does well in practice.

A simple initialization procedure for $k$-means is both effective and gives provable guarantees.

Much of the theoretical machinery around $k$-means works for the generalization to Bregman divergences.

New and interesting questions on the relationship between the target clustering and cost measures used to get near it: ways of subverting NP-hardness.
Thank You

Slides for this tutorial can be found at

http://www.cs.utah.edu/~suresh/web/2010/05/08/
new-developments-in-the-theory-of-clustering-tutorial/

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