Fast and Accurate $k$-means for Large Data Sets

Michael Shindler    Alex Wong    Adam Meyerson
K-means Clustering

\[ \text{cost}(F) = \sum_{i \in X} \min_{j \in F} \|X_i - X_j\|^2 \]

“facilities” or “centers” or “means”
Algorithms for solving $k$-means

- Standard Algorithm (Lloyd 57)
  - Can have cost arbitrarily worse than optimal (Arthur and Vassilvitskii, 07)
  - Can take exponential time (Vattani, 11)

- Polynomial time algorithms for $k$-means
  - Bound ratio of (algorithm cost) / (optimal cost)
  - Best ratio is $9 + \varepsilon$ due to (Kanungo et al, 02)

- These do not work for streaming setting
K-means for Large Datasets

• Want good $k$-means solution
  – Without random access to full data
  – Without using much memory
  – Without using much time
Streaming $k$-means

When done:
If more than $k$ facilities,
Use normal $k$-means to consolidate

Probability $\propto$ distance
## Improvements/Contributions

<table>
<thead>
<tr>
<th></th>
<th>Braverman <em>et al</em> (SODA 2011)</th>
<th>This Work</th>
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</thead>
<tbody>
<tr>
<td><strong>Memory Requirement</strong></td>
<td>1623 $k \log n$</td>
<td>Any $\Omega(k \log n)$ (including 1 $k \log n$)</td>
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<tr>
<td><strong>Cost Guarantee</strong></td>
<td>$O(1)$ 60,498</td>
<td>$O(1)$ 17</td>
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<td>(cost ratio against best)</td>
<td></td>
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<tr>
<td><strong>If too many facilities</strong></td>
<td>Complicated matching</td>
<td>Simple re-evaluation</td>
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<td>before finishing stream?</td>
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<td><strong>Optimized</strong></td>
<td>$O(nk \log n)$ Large lead constant</td>
<td>$o(nk)$ Less than $\theta(nk)$</td>
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<tr>
<td><strong>runtime</strong></td>
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More relevant algorithms for streaming $k$-means

- **Divide and Conquer** (Ailon, Jaiswal, and Monteleoni, NIPS 09)
  
  - Read $M$ points into memory
  
  - Compute and store weighted representative points
  
  - Repeat until stream exhausted
  
  - Compute $k$-means on stored representatives

- **StreamKM++** (Ackermann et al, ALENEX 10)
  
  - Compute a weighted representative sample of stream
  
  - Solve $k$-means on sample
  
  - Based on *core set* paradigm
    
    - For current best theoretical treatment, see (Chen 09)
Experimental Setup

• Compare to others with equal memory

• Metrics:
  – Cost of solution (squared error)
  – Time to compute solution

• Examples in this talk are from UCI “Census 1990” dataset
  – 2,458,285 points in 68 dimensions
  – Seeking $k = 12$ clusters
Time to Compute Solution

Ours ≈ fastest
Cost (Summed Squared Distances)

With enough memory, Ours is best
Bottleneck in Algorithm Runtime

- **Choose Random Vector** $\omega \in [0,1)^d$
- **O(κ) time** (if κ facilities)
- **Identify Two Nearest Neighbors** $O(\log \kappa)$
Compute Actual Distance to Those Neighbors
Substantially Faster
Cost change is (usually) minor
Conclusion

• Fast streaming $k$-means algorithm
  – Substantial Speedup

• Provides good quality clustering
  – Best $O(1)$ cost guarantee among poly-time streaming algorithms

• Source Code available from
  http://web.engr.oregonstate.edu/~shindler/
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Additional Slides
Room for Improvement

• [BMO+11] should be fast and straightforward
• However:
  – Actual memory requirements are high
    • $O(k \log n)$ memory great in limit
    • Facility cap of $\kappa = 1623 \ k \log n$
  – Constant approximation bound is high
    • Constant is tens of thousands
  – End-of-phase conditions are complicated
End-of-phase conditions

• End-of-phase in [BMO+11]
  – “Phase” is reading data until $f$ too low
  – When done, need to re-evaluate facilities and increase $f$
  – Performed maximal matching as part of this
  – Guaranteed no more than $\frac{n}{k \log n}$ phases

• Simpler phase transitions
  – Transition only on facility count
  – Increase $f$
  – Push facilities (weighted) back to stream
  – Continue reading stream, starting at those
  – Faster, no guarantee of phase count
Memory Requirement

• [BMO+11] : facility cap of $1623 \ k \ \log n$
• Great as an asymptotic bound
• Quite large in practice
• Instead, we will allow any $\kappa$ facilities
• Facility count $\kappa$ can be any in $\Omega(k \ \log n)$
• Will demonstrate that $\kappa = k \ \log n$ works well
Approximation Bound

• Ratio of cost of solution vs optimal
• Approximation factor in [BMO+11] is 60,498
• We achieve a bound of 17
Algorithm: Spot the Bottleneck

Consolidate facilities
Return final $k$ means

Push weighted facilities to stream

Read next point?

Have $k$ facilities?

Make it a new facility

Increase “weight” of nearest
Do not “remember” this point

Probability $\delta/f$?

Consolidate facilities
Return final $k$ means

Push weighted facilities to stream

Have $k$ facilities?

Make it a new facility

There is one

Measure $\delta = \text{distance to nearest facility}$

no

yes

done

fewer
Algorithm: Spot the Bottleneck

1. Read next point?
   - done

2. Have $k$ facilities?
   - yes
     - Push weighted facilities to stream
   - no
     - Make it a new facility
       - Probability $\delta/f$?
         - yes
           - Increase “weight” of nearest
distance to nearest facility
         - no
           - Measuring $\delta = \text{distance to nearest facility}$
Bottleneck: Finding Nearest Facility

• Use approximate nearest neighbor algorithms
• To achieve guarantee:
  – Techniques from hashing and metric embedding
  – Look up is $O(\log n(\log k + \log \log n))$
• MAIN RESULT:
  – Algorithm runtime is $o(nk)$ for most values of $k$
  – (Computing cost given solution takes $\Theta(nk)$)
Bottleneck: Finding nearest Facility

- Fast practical implementation:
  - Select random point \( \omega \in [0,1)^d \)
  - Store facilities sorted by inner product with \( \omega \)
  - To find “nearest” facility to \( x \):
    - Find \( a, b \):
      - \( a \cdot \omega \leq x \cdot \omega \leq b \cdot \omega \)
    - Use closer of \((a,b)\)
Bottleneck in Algorithm Runtime