Constrained K-means Clustering with Background Knowledge

paper by

Kiri Wagstaff, Claire Cardie,

Seth Rogers and Stefan Schroedl

presented by

Siddharth Patwardhan

An Overview of the Talk

- Introduction to clustering and the common trends.
- The basic k-means algorithm.
- Applying constraints based on background knowledge.
- How do we evaluate?
- Experiment using artificial constraints.
- A GPS lane finding experiment.
- Related work.
- Conclusions.

Clustering!

- An unsupervised method for data analysis.
- Grouping of data with some notion of "similarity".
- Uses just the data to determine which of the data points look alike.
- New instances of data are assigned to the closest cluster.

Background Knowledge

- Traditional clustering algorithms don't use any background knowledge about the data in the clusters.
- If domain knowledge told us…
  - Two data points are part of the same class.
  - Or two data points are in different classes.
- … could we improve the clusters formed?

The K-means Algorithm

- Automatically partitions data points into k groups.
- Starts with k initial "cluster centers", iteratively assigns points to clusters and updates the "cluster centers".
- Converges when there is no further change in assignment of points to clusters.

Using Background Knowledge

- Two types of constraints based on the domain knowledge.
- **Must-link** constraints specify that two instances must be in the same cluster.
- **Cannot-link** constraints specify that two instances cannot be in the same cluster.

The Constrained K-means Algorithm

(1) Initialize the *k* cluster centers.

(2) For each data point d_i, assign d_i to its closest cluster **such that none of the constraints are violated.** If no such cluster exists, clustering fails.

(3) Update the cluster centers.

(4) Iterate (2) and (3) till convergence.

Testing Constraint Violation

- The distance of a data point *d* to each of the cluster-centers is computed.
- Constraint violation for *d* is tested for each cluster in ascending order of distance of *d* from the cluster-center.

Testing Constraint Violation

- For a cluster *C*, from the data-points that have been assigned to clusters, if the data points that "must-link" to *d* are not in *C*, then the must-link constraint for *d* is violated.
- For a cluster *C*, if any of the data points that "cannot-link" to *d* are in *C*, then the cannot-link constraint for *d* is violated.

Evaluating Clusters

- *Rand Index* used to measure the agreement between partitions.
- In this case the partitions are
  - that formed by the clustering.
  - that specified by the data point labels.
- Accuracy measured for the entire data set and for a "held-out" test set (subset of the non-constrained data point) using a 10-fold cross validation.

More Evaluation

- The constraints can be viewed as a partition of the data points and thus can be evaluated using the *Rand Index*.
- The accuracy of the partition of just the constraints determine how good the constraints by themselves are at forming the clusters.
- This analysis consequently determines how well the domain knowledge by itself clusters the data.

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An Experiment using Artificial Constraints

- Used 6 well-known test sets from the UCI repository to test the performance of the constrained k-means algorithm.
- Tested basic k-means on each data set to provide a baseline for comparison.
- Tested the constrained k-means on each data set, varying the number of constraints.

Generating the Constraints

- Randomly select a pair of data points.
- If the two points have the same label, create a must-link constraint between them.
- If the two points have a different label, create a cannot-link constraint between them.
- Repeat the above process *n* times to generate *n* constraints.

The *soybean* Data Set

- 47 instances, 35 attributes, 4 classes.
- Unconstrained k-means achieves an accuracy of 87 %.
- Accuracy of the constraints alone: 48 %.
- Accuracy of constrained k-means on entire data set increases with the number of constraints up to 99 %, with 100 random constraints.
- With the held-out data set it increases at almost the same rate to 98 %.

The *soybean* Data Set

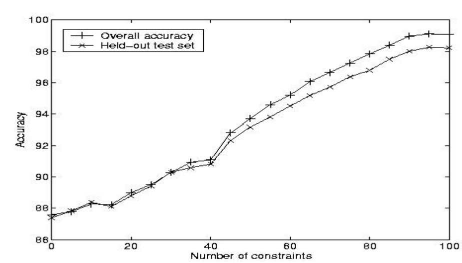

Figure 1. COP-KMEANS results on soybean

The *mushroom* Data Set

- 50 instances, 21 attributes, 2 classes.
- Unconstrained k-means achieves an accuracy of 69 %.
- Accuracy of the constraints alone: 73 %.
- Accuracy of constrained k-means on entire data set increases with the number of constraints up to 96 %, with 100 random constraints.
- With the held-out data set it increases at almost the same rate to 83 %.

The *mushroom* Data Set

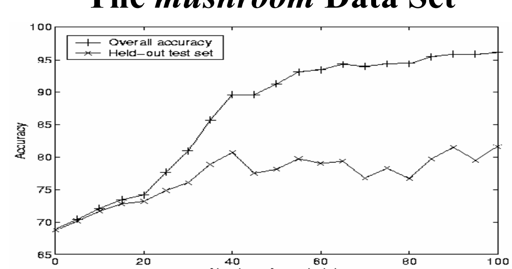

Figure 2. COP-KMEANS results on mushroom

Making a Point

- On the other data sets too (part-of-speech, tic-tac-toe, iris, wine) the overall accuracy rose sharply into the 90s.
- Held-out accuracy increased only marginally.
- Improvement in clustering accuracy depends on the data set in question.
- Improvements can be observed on unconstrained instances, if constraints are generalizable to the full data set.

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GPS Lane Finding Experiment

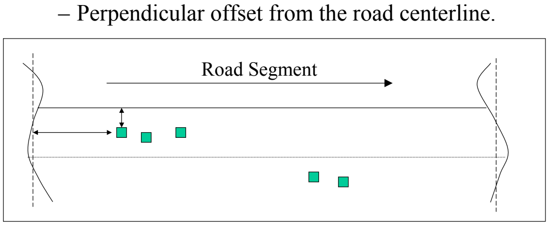
- Representing the problem as a clustering problem.
- Extracting constraints from background knowledge.
- Applying k-means with and without using constraints.
- Comparison of the results.

Lane Finding

- Clustering data points gathered from GPS systems.
- Clusters indicate lanes – densely traveled spaces.
- Can be used to alert drivers drifting from their lane.

Data Description

- Each data point represented by two features:
  - Distance along the road segment.
  - Perpendicular offset from the road centerline.



Data Description

- For evaluation purposes, each data point is also classified by the lane in which the it lies.
- Data collected once per second from several drivers with GPS receivers.
- Drivers specified which lane they were in to help label each data point.

The Background Knowledge

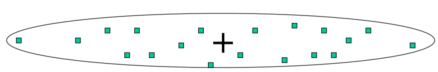
- Domain-specific heuristics – **trace contiguity** and **maximum separation**.
- Trace contiguity: In the absence of lane changes, all points from a vehicle should be in the same cluster.
- Maximum separation: If two points are at least 4m apart vertically, they cannot be in the same lane.

Applying the Knowledge

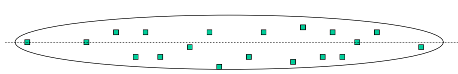
- Using trace contiguity – Data points generated from the same vehicle that didn't change lanes in a particular segment constrained to the same cluster.
- Using maximum separation – Data points separated by a distance greater than 4m vertically are constrained to be in different clusters.

Cluster-Center Representation

Rather than a point:



Represented as a line:



Selecting the value of *k*

- Used a second measure to compute the best value of k.
- Randomly select a value of k from 1 to 5 and apply the clustering algorithm.
- Minimize:

$$\left(\frac{\sum_i dist(d_i, d_i \cdot clusterCenter}{n}\right) \times k^2$$

Selecting the value of *k*

- Selected the best k across 30 trials each.
- The basic k-means never chose the correct value for k.
- The COP-KMEANS selected the correct value for k for all but one road segment.

The Data

- 20 data sets, i.e. 20 road segments.
- Different number of lanes in each segment – i.e. different k for each data set.
- Number of data points for each segment ranging from 115 to 1160.
- Significantly larger than previous experiment.

Results

- Average accuracy of unconstrained k-means: 58.0 %.
- Un-constrained k-means attained a maximum accuracy of 75 % .
- Selected the wrong value for *k* for all sets.

- Average accuracy of constrained k-means: 98.6 %.
- Constrained k-means attained 100 % accuracy for 17 out of the 20 data sets.
- Selected the wrong value for *k* for one set.

Results

- Experiment specifying the correct value of *k* to the unconstrained k-means on data set #6 showed that it still performs poorly.
- Seeks compact spherical clusters.
- Clusters formed span multiple lanes.

Conclusions

- General method to incorporate background knowledge in clustering by using instance level constraints.
- Successfully applied to a real world problem.
- Scalable to large data sets.

More Conclusions

- Might be argued that k-means is fundamentally a poor choice of algorithm for the task.
- The constraints by themselves do not achieve good clustering.
- Combination of the constraints and a poor clustering algorithm can boost its performance.

Order-sensitive Clustering

- A downside of the method is that the clustering is sensitive to the order of assignment of points to the clusters.
- A poor decision at the start can result in can result in poor clusters or “no possible clusters” later.
- Ideally, backtracking could be incorporated in the latter case.

Related Work – Some Other Techniques

- Some agglomerative clustering algorithms use contiguity constraints.
- These cover the entire data set and cannot handle partial constraints.
- No accommodation for constraints to separate data items.

Related Work

- K-means can evolve empty clusters.
- This will result in fewer than *k* clusters.
- By imposing a minimum size on each cluster, this can be avoided.
- This is a cluster level constraint.
- Like instance level constraints, cluster level constraints can be used to incorporate domain knowledge.

Putting to the Test

- Using constrained k-means in text clustering – clustering contexts with the same sense of a target word.
- Using background knowledge from sources like dictionaries and statistical information from large corpora to generate constraints.
- Using background knowledge to select the initial *k* points.

Constrained K-means clustering with background knowledge

By: Kiri Wagstaff, Claire Cardie
Seth Rogers , Stefan Schroedl

Presented by : Siddharth Patwardhan
Comments by : Sachin sharma

Soft Constraints (preferences)…

- Previously defined two *Hard Constraints*
  - **must link**
  - **cannot link**
- Augmenting strength factor to each relation
  → soft constraints or preferences

e.g. $<d_i,d_k,s>$

0 <= |s| <= 1

Soft constraints , cont…

- Subsumes both ***soft*** and ***hard*** constraints
- **s** , +ve values : group together
  -ve values : *don't* group together

$<d_i,d_k,1>$ == must link hard constraint

$<d_i,d_k,-1>$ == cannot link hard constraint

$< d_i,d_k,0>$ == don't care hard constraint

Soft constraint closure

for all i, j, k : given	produce
$d_i =_m d_J$ and $d_J =_m d_k$	$d_i =_m d_k$
$d_i =_m d_J$ and $d_J !=_c d_k$	$d_i !=_c d_k$
$d_i !=_c d_J$ and $d_J =_m d_k$	$d_i !=_c d_k$
for all i, j, k : given	**produce**
$<d_i,d_J,s1>$ $< d_J,d_k,s2>$	$< d_i, d_k,\min(s1,s2)>$
$<d_i,d_J,s1>$ $< d_J,d_k,-s2>$	$< d_i, d_k,-\min(s1,s2)>$
$<d_i,d_J,-s1>$ $< d_J,d_k,s2>$	$< d_i, d_k,-\min(s1,s2)>$

If both constraints negative ....conclusion ?..?..?

Constrained K-means Clustering with background Knowledge

Presented by Siddhartha Patwardhan

Comments

Sweta Sinha

Overview

- Integration of Background knowledge in constrained K-means clustering
- Background knowledge incorporated in the form of instance level constraints
- Variant of k-means algorithm
- Significant improvements in accuracy

Evaluation Method

- Dataset used for evaluation has label for each instance
- Rand index used to calculate measure of agreement between cluster obtained and the actual classification

  Let us take dataset with 6 instances {a,b,c,d,e,f}

  Clusters by clustering algorithm { (a,b,c), (d,e,f)

  Actual classification {(a,b), (c,d,e), (f)}

Point pair	ab	ac	ad	ae	af	bc	bd	be	bf	cd	ce	cf	de	df	ef	Σ
together	*												*			2
separate			*	*	*		*	*	*			*				7
mixed		*				*				*	*			*	*	6

Total no of pairs = n*(n-1)/2 = 15

Similarity = (2+7)/15 = 0.6