An implementation of the relational k-means algorithm

Balázs Szalkai Eötvös Loránd University, Budapest, Hungary

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Abstract

A $C\sharp$ implementation of a generalized k-means variant called *relational k-means* is described here. Relational k-means is a generalization of the well-known k-means clustering method which works for non-Euclidean scenarios as well. The input is an arbitrary distance matrix, as opposed to the traditional k-means method, where the clustered objects need to be identified with vectors.

1 Introduction

Suppose that we are given a set of data points $p_1, ...p_n \in \mathbb{R}^d$ and a number of clusters N. We would like assort these data points "optimally" into N clusters. For each point p_i let z_i denote the center of gravity of the cluster p_i is assigned to. We call the z_i vectors centroids. The standard k-means method [2] attempts to produce such a clustering of the data points that the sum of squared centroid distances $\sum_{i=1}^{n} ||p_i - z_i||^2$ is minimized.

The main difficulty of this method is that it requires the data points to be the elements of a Euclidean space, since we need to average the data points somehow. A generalization of k-means called *relational k-means* has been proposed [3] to address this issue. This generalized k-means variant does not require the data points to be vectors.

Instead, the data points $p_1, ...p_n$ can form an abstract set S with a completely arbitrary distance function $f: S \times S \to [0, \infty)$. We only require that f is symmetrical, and $f(p_i, p_i) = 0$ for all $p_i \in S$. Note that f need not even satisfy the triangle inequality.

2 Relational k-means

First, we provide a brief outline of the algorithm. Let $A \in \mathbb{R}^{n \times n}$ be the squared distance matrix. That is, $A_{ij} = f(p_i, p_j)^2$. The algorithm starts with some initial clustering and improves it by repeatedly performing an iteration step. The algorithm stops if the last

iteration did not decrease the *value* of the clustering (defined below). Of course, if the iteration increased the value of the clustering, the algorithm reverts the last iteration.

Now we describe the algorithm in detail. At any time during execution, let $S_1, ... S_N \subset S$ denote the clusters. For each data point p_i , let $\ell(p_i)$ denote the index of the cluster p_i is assigned to. Let $e_i \in \mathbb{R}^n$ denote the ith standard basis vector, and, for $i \in \{1, ... n\}$ and $j \in \{1, ... N\}$ let $v_{ij} := \frac{1}{|S_j|} \sum_{k \in S_j} e_k - e_i$. Let us call the quantity $q_{ij} := -\frac{1}{2} v_{ij}^{\mathsf{T}} A v_{ij}$ the squared centroid distance corresponding to the point p_i and the cluster S_j .

In [3] it is observed that, if the distance function is derived from a Euclidean representation of the data points, then q_{ij} equals to the squared distance of p_i and the center of gravity of S_j . Thus q_{ij} is indeed an extension of the classical notion of squared centroid distances.

Define the value of a clustering as $\sum_{i=1}^{n} q_{i\ell i}$. We say that a clustering is better than another one if and only if its value is less than the value of the other clustering.

The relational k-means algorithm takes an initial clustering (e.g. a random one), and improves it through repeated applications of an iteration step which reclusters the data points. The iteration step simply reassigns each data point to the cluster which minimized the squared centroid distance in the previous clustering. If the value of clustering does not decrease through the reassignment, then the reassignment is undone and the algorithm stops.

In the non-Euclidean case there might be scenarios when an iteration actually worsens the clustering. Should this peculiar behavior be undesirable, it can be avoided by "stretching" the distance matrix and thus making it Euclidean.

Stretching means replacing A with $A + \beta(J - I)$, where J is the matrix whose entries are all 1's, I is the identity matrix, and $\beta \geq 0$ is the smallest real number for which $A + \beta(J - I)$ is a Euclidean squared distance matrix, i.e. it equals to the squared distance matrix of some n vectors. It can be easily deducted that such a β exists. This method is called β -spread transformation (see [1]).

The algorithm is thus as follows:

- Start with some clustering, e.g. a random one
- Calculate the value of the current clustering and store it in V_1
- For each p_i data point, calculate and store the squared centroid distances $q_{i1}, ... q_{iN}$
- Reassign each p_i data point to the cluster that yielded the smallest squared centroid distance in the previous step
- Calculate the value of the current clustering and store it in V_2
- If $V_2 \geq V_1$, then undo the previous reassignment and stop
- Go to line number 2

3 Time complexity

The algorithm is clearly finite because it gradually decreases the value of the current clustering and the number of different clusterings is finite. Each iteration step can easily be implemented in $\mathcal{O}(n^3)$ time: for each data point, we need to calculate N quadratic forms, which can be done in $n \sum_{j=1}^{N} |S_j|^2 \leq n^3$ time. This is unfortunately too slow for practical applications.

However, this can be improved down to $\mathcal{O}(n^2)$. The squared centroid distances can be transformed as follows (using $A_{ii} = 0$):

$$q_{ij} = -\frac{1}{2} \left(\frac{1}{|S_j|} \sum_{k \in S_j} e_k - e_i \right)^{\top} A \left(\frac{1}{|S_j|} \sum_{k \in S_j} e_k - e_i \right) = -\frac{1}{2|S_j|^2} \sum_{a,b \in S_j} A_{ab} + \frac{1}{|S_j|} \sum_{k \in S_j} A_{ik}.$$

Here the first summand is independent of i and thus needs to be calculated for each cluster only once per iteration. On the other hand, the second summand can be calculated in $\mathcal{O}(|S_j|)$ time. To sum up, the amount of arithmetic operations per iteration is at most constant times $\sum_{j=1}^{N} |S_j|^2 + n \sum_{j=1}^{N} |S_j| \leq 2n^2$.

The current implementation makes several attempts to find a better clustering. In each attempt, the full relational k-means algorithm is run, starting from a new random clustering. Every attempt has the possibility to produce a clustering which is better than the best one among the previous attempts. If the sofar best clustering has not been improved in the last K attempts (where K is a parameter), then it is assumed that the clustering which is currently the best is not too far from the optimum, and the program execution stops.

Attempts do not depend on each other's result and do not modify shared resources (apart from a shared random generator). Our implementation uses Parallel.For for launching multiple attempts at once. The number of parallel threads can be customized via a command-line switch, and by default equals to the number of logical processors. This results in near 100% CPU utilization. Launching less than C threads allows leaving some CPU time for other processes.

4 Test results and conclusion

We implemented the above algorithm in $C\sharp$ and run the program on a set of >1000 proteins with a Levenshtein-like distance function. The value of K (maximum allowed number of failed attempts, i.e. the "bad luck streak") was 20, and the value of N (number of clusters) was 10. The testing was done on an average dual core laptop computer and finished in 30..60 seconds. This proves that relational k-means can be implemented in a way efficient enough to be applied to real-world datasets.

Since the program is almost fully parallelized, we could expect it to finish in <8 seconds for the same dataset on a 16-core machine. Note that the total runtime is proportional

to the number of attempts made, which is highly variable due to the random nature of the algorithm.

A C++ implementation could further reduce execution time. According to our estimate, it could make the program cca. twice as fast.

5 Attachments

5.1 Program source code in C^{\sharp}

```
//Generalized k-means
//Copyright (C) 2013 Balazs Szalkai
//If you use this program in your research, please cite the following article:
//B. Szalkai: An implementation of the relational k-means algorithm. ArXiv e-prints, 2013.
//This program is free software: you can redistribute it and/or modify //it under the terms of the GNU General Public License as published by
//the Free Software Foundation, either version 3 of the License, or
\ensuremath{//}\mbox{(at your option)} any later version.
//This program is distributed in the hope that it will be useful, //but WITHOUT ANY WARRANTY; without even the implied warranty of //MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
//GNU General Public License for more details.
//You should have received a copy of the GNU General Public License
//along with this program. If not, see <a href="http://www.gnu.org/licenses/">http://www.gnu.org/licenses/</a>
using System.Collections.Generic;
using System.Globalization;
using System.IO;
using System.Reflection;
using System. Threading;
using System. Threading. Tasks;
namespace GeneralizedKMeans
  static class Utils
     public static double Sqr(double x)
       return x * x;
  class DistanceMatrix
     public string[] Name;
     public double[,] SqrDistance;
     public DistanceMatrix()
       Resize(0);
     public void Resize(int NewCount)
       Count = NewCount;
       Name = new string[Count];
       SqrDistance = new double[Count, Count];
     public void Load(string fn)
       string[] lines = File.ReadAllLines(fn);
       Resize(Array.IndexOf(lines, "//"));
       for (int i = 0; i < Count; i++)
          Name[i] = lines[i].Trim();
          string[] distLine = lines[Count + 1 + i].Split(';');
for (int j = 0; j < Count; j++)
    SqrDistance[i, j] = Utils.Sqr(double.Parse(distLine[j].Trim(), CultureInfo.InvariantCulture));</pre>
   class CentroidDistance
    public Clusters Clusters;
```

```
double ☐ AdditiveConstant:
  public CentroidDistance(Clusters clusters)
    Clusters = clusters;
  // Call this before using the other members functions
  public void Initialize()
    // calculate additive constants for clusters
    AdditiveConstant = new double[Clusters.Count];
for (int cluster = 0; cluster < Clusters.Count; cluster++)
       var objects = Clusters.ClusterToObjects[cluster];
       foreach (var i in objects)
         foreach (var j in objects)
       x += Clusters.Matrix.SqrDistance[i, j];
AdditiveConstant[cluster] = -x / (2 * Utils.Sqr((double)objects.Count));
  // Calculates a squared centroid distance
 public double CalculateSqrDist(int obj, int cluster)
    var objects = Clusters.ClusterToObjects[cluster];
    double x = 0;
    foreach (int j in objects) x += Clusters.Matrix.SqrDistance[obj, j];
double dist = AdditiveConstant[cluster] + x / objects.Count;
    return dist:
  public int GetNearestCluster(int obj)
    int nearestCluster = -1;
double minSqrDist = 0;
    for (int cluster = 0; cluster < Clusters.Count; cluster++)
       double sqrDist = CalculateSqrDist(obj, cluster);
if (nearestCluster < 0 || sqrDist < minSqrDist)</pre>
         minSqrDist = sqrDist;
         nearestCluster = cluster;
    return nearestCluster;
  public double GetClusteringValue()
    double result = 0;
for (int i = 0; i < Clusters.Matrix.Count; i++)
   result += CalculateSqrDist(i, Clusters.ObjectToCluster[i]);</pre>
class Clusters
  public DistanceMatrix Matrix;
  public int Count:
 public int[] ObjectToCluster;
public List<int>[] ClusterToObjects;
  private CentroidDistance cd;
  public Clusters(DistanceMatrix matrix, int count)
    Matrix = matrix;
    Count = count;
    ObjectToCluster = new int[Matrix.Count];
ClusterToObjects = new List<int>[Count];
for (int i = 0; i < Count; i++) ClusterToObjects[i] = new List<int>();
    cd = new CentroidDistance(this);
    Randomize();
  private static Random Rand = new Random();
  public void Randomize()
    for (int i = 0; i < Count; i++) ClusterToObjects[i].Clear();</pre>
```

```
for (int i = 0; i < Matrix.Count; i++)
           int cluster = Rand.Next(Count);
           ObjectToCluster[i] = cluster;
           ClusterToObjects[cluster].Add(i);
   private void Make_ClusterToObjects()
{
      for (int cluster = 0; cluster < Count; cluster++)
      ClusterToObjects[cluster].Clear();
for (int i = 0; i < Matrix.Count; i++)</pre>
        ClusterToObjects[ObjectToCluster[i]].Add(i);
    // Returns how many objects have changed cluster
    public int Iterate()
      int changed = 0;
cd.Initialize();
      \ensuremath{//} find the nearest centroid for the objects
      int[] New_ObjectToCluster = new int[Matrix.Count];
for (int i = 0; i < Matrix.Count; i++)</pre>
        New_ObjectToCluster[i] = cd.GetNearestCluster(i);
if (New_ObjectToCluster[i] != ObjectToCluster[i]) changed+++;
      // update the configuration
      double oldValue = GetValue();
      int[] Old_ObjectToCluster = ObjectToCluster;
      ObjectToCluster = New_ObjectToCluster;
      Make_ClusterToObjects();
      double newValue = GetValue();
      /\!/ clustering got worse (this is possible with some distance matrices) or stayed the same? if (oldValue <= newValue)
        // undo iteration
ObjectToCluster = Old_ObjectToCluster;
        Make_ClusterToObjects();
        return 0;
   return changed;
   public double GetValue()
      cd.Initialize();
     return cd.GetClusteringValue();
   public void Dump(TextWriter w)
      w.WriteLine(Matrix.Count + ";objects");
     w.WriteLine(Count + ";clusters");
w.WriteLine(GetValue() + ";value");
for (int i = 0; i < Matrix.Count; i++)
w.WriteLine(ObjectToCluster[i] + ";<-;" + Matrix.Name[i]);</pre>
      for (int cluster = 0; cluster < Count; cluster++)
        w.Write(cluster+":->"):
        foreach (var i in ClusterToObjects[cluster]) w.Write(";" + Matrix.Name[i]);
        w.WriteLine():
     }
}
 class Program
    const int maxBadLuckStreak_Default = 100;
    void Run(Dictionary<string,string> args)
      string inputFile = args["i"];
      int nClusters = int.Parse(args["n"]);
      Int. nctusers - Int.raise(args in j), string outputFile = args.ContainsKey("o") ? args["o"] : null; int maxBadLuckStreak = args.ContainsKey("m") ? int.Parse(args["m"]) : maxBadLuckStreak_Default;
      int nThreads = args.ContainsKey("t") ? int.Parse(args["t"]) : 0;
      if (nThreads <= 0) nThreads += Environment.ProcessorCount:
      nThreads = Math.Max(1, nThreads);
      DistanceMatrix m = new DistanceMatrix();
      m.Load(inputFile);
      Clusters bestClusters = new Clusters(m. nClusters):
      int badLuckStreak = 0:
```

```
int blockId = 0;
 Clusters[] clustersArray = new Clusters[nThreads];
  while (true)
    Parallel.For(0, nThreads, i =>
         Console.WriteLine("Attempt " + (nThreads*blockId + i + 1));
Clusters c = new Clusters(m, nClusters);
while (true)
           Console.WriteLine("Current value is " + c.GetValue());
if (c.Iterate() == 0) break;
         clustersArray[i] = c;
      }):
    Console.WriteLine();
    for (int i = 0: i < nThreads: i++)
      Clusters c = clustersArray[i];
if (c.GetValue() < bestClusters.GetValue())</pre>
         Console.WriteLine("Found a better clustering");
         bestClusters = c:
        badLuckStreak = 0;
       else badLuckStreak++;
    Console.WriteLine();
   if (badLuckStreak >= maxBadLuckStreak) break;
 Console.WriteLine("Final value is " + bestClusters.GetValue());
  Console.WriteLine();
 // output the clustering
if (outputFile != null)
    using (StreamWriter sw = new StreamWriter(outputFile)) bestClusters.Dump(sw);
 else bestClusters.Dump(Console.Out);
static void Main(string[] args)
 \label{lem:console.WriteLine("Generalized k-means, (c) 2013 Bal\x00E1zs Szalkai"); \\ Console.WriteLine("Released under GNU GPL version 3"); \\
 Console.WriteLine("If you use the program in your research, please cite the following article:");
Console.WriteLine("B. Szalkai: An implementation of the relational k-means algorithm. ArXiv e-prints, 2013.");
 if (args.Length == 0)
   Dictionary<string, string> parsedArgs = new Dictionary<string,string>();
for (int i = 0; i + 1 < args.Length; i += 2) parsedArgs[args[i].ToLower()] = args[i + 1];</pre>
 if (!parsedArgs.ContainsKey("i"))
    Console.WriteLine("Missing argument: input file");
    return;
 if (!parsedArgs.ContainsKey("n"))
    Console.WriteLine("Missing argument: number of clusters");
 new Program().Run(parsedArgs);
```

5.2 Example input

The first n lines of the input contain the names of the objects which need to be clustered. Then a line containing two slashes follows. After that, a matrix containing the pairwise distances is listed in semicolon-separated CSV format. Fractional distances must be input with the dot character (.) as decimal separator.

References

- [1] Richard J. Hathaway and James C. Bezdek. Nerf c-means: Non-euclidean relational fuzzy clustering. *Pattern Recognition*, 27(3):429–437, 1994.
- [2] J. B. MacQueen. Some methods for classification and analysis of multivariate observations. In L. M. Le Cam and J. Neyman, editors, *Proceedings of the 5th Berkeley Symposium on Mathematical Statistics and Probability*, pages 281–297. University of California Press, 1967.
- [3] B. Szalkai. Generalizing k-means for an arbitrary distance matrix. $ArXiv\ e\text{-}prints\ http://arxiv.org/abs/1303.6001$, March 2013.