Data Clustering using Particle Swarm Optimization

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Agenda

- Standard K-means and main drawbacks
- The Particle Swarm Optimization [PSO] Algorithm
- Applying PSO to clustering
- Hybrid K-means/PSO algorithm
- Matlab example and some results
- References
K-means and drawbacks

- **K-means**
  - K-Means is one of the most popular clustering algorithms, **and it is easy to implement**
  - It seeks to minimize the sum of squared errors with an iterative optimization
  - At every iteration, it moves the data centroids toward the closer cluster until no point can move anymore

- **Drawbacks**
  - It implements a Hill-climbing procedure
  - Highly dependent on the choice of K
  - **Sensitive to initialization: how do we choose the initial partitions?**

References: Prof. E. Messina, Lesson2 http://www.mind.disco.unimib.it/gallery/index.asp?cat=330&level=2
Particle Swarm Optimization Algorithm

- Optimization Algorithm
  - iterative search process modeled after the social behavior of a bird flock
  - each particle represents a potential solution

- Goal
  - find the “best” particle position i.e. best in the evaluation of a given fitness (objective) function

- Q: how to cluster using PSO?
The PSO algorithm code

How to implement the algorithm?

We wrote the full code of PSO using Matlab, in less than 100 lines of code!

The code will be available in my personal page in the IRALAB website
www.ira.disco.unimib.it/people/ballardini-augusto-luis/

Let we see the algorithm pseudo-code

1. Initialize each particle to contain $N_c$ randomly selected cluster centroids.

2. For $t = 1$ to $t_{max}$ do
   (a) For each particle $i$ do
      (b) For each data vector $z_p$
         i. calculate the Euclidean distance $d(z_p, m_{ij})$ to all cluster centroids $C_{ij}$
         ii. assign $z_p$ to cluster $C_{ij}$ such that $d(z_p, m_{ij}) = \min_{v=1,...,N_c} \{d(z_p, m_{iv})\}$
         iii. calculate the fitness using equation (8)
   (c) Update the global best and local best positions
   (d) Update the cluster centroids using equations (3) and (4).
Rules in the PSO algorithm (1)

Each particle $i$ maintains:
- $x_i$, as the current position (currently initialized randomly)
- $v_i$, as the current velocity (currently initialized randomly)
- $y_i$, as the personal best position

Each particle’s position is adjusted according to
- $v_{i,k}(t+1) = w * v_{i,k}(t) + c_1 * r_{1,k}(t) * (y_{i,k}(t) - x_{i,k}(t)) + c_2 * r_{2,k}(t) * (\hat{y}_{i,k}(t) - x_{i,k}(t))$
- $x_{i}(t+1) = x_{i}(t) + v_{i,k}(t+1)$
Rules in the PSO algorithm (2)

- How to calculate the ‘best’ position?

\[ y_i(t+1) = \begin{cases} 
  y_i(t) & \text{if } f(x_i(t+1)) \geq f(y_i(t)) \\
  x_i(t+1) & \text{if } f(x_i(t+1)) < f(y_i(t)) 
\end{cases} \]

- A swarm represents a number of candidate clusterings (cluster centroids) for the input; the fitness of these particles is measured as the quantization error (over all the cluster centroids of the particle)!

\[
J_e = \frac{\sum_{j=1}^{N_c} \left[ \sum_{\forall z_p \in C_{ij}} d(z_p, m_j) / |C_{ij}| \right]}{N_c}
\]
Rules *(explained)* in the PSO algorithm

*This is the swarm: n=2 particles, each one has k=2 centroids with 2 classes (x and y)*
Rules (explained) in the PSO algorithm

Position vectors of the swarm

\[
\begin{bmatrix}
    x_a & y_a \\
    x_b & y_b
\end{bmatrix}
\]

Velocity vectors of the swarm

\[
\begin{bmatrix}
    v_{ax} & v_{ay} \\
    v_{bx} & v_{by}
\end{bmatrix}
\]

BEST position of the swarm

\[
\begin{bmatrix}
    x_a & y_a \\
    x_b & y_b
\end{bmatrix}
\]

GLOBAL BEST position of the swarm

\[
\begin{bmatrix}
    x_a & y_a \\
    x_b & y_b
\end{bmatrix}
\]
Rules (explained) in the PSO algorithm

- Initialization with Random Poses (PSO)
- Compute Distances
- Assign inputs to Clusters
- Evaluate Fitness
- Update Cluster Centroids
- Update Local Best and Global Best
Rules (explained) in the PSO algorithm

How to calculate the position of the particle (already initialized with random values)

Please, consider \{w, c1, c2\} as constants and \{r1, r2\} as values sampled from U(0,1)

- **1st calculate new velocity of the particle**
  \[ v_{i,k} (t+1) = w \times v_{i,k} (t) + c_1 \times r_{1,k}(t) \times (y_{i,k}(t) - x_{i,k}(t)) + c_2 \times r_{2,k}(t) \times (\hat{y}_{i,k}(t) - x_{i,k}(t)) \]

  - **inertia**
  - **cognitive component**
  - **social component**

  *cognitive* = distance of the particle from its personal best position

  *social* = distance of the particle from the best particle found so far (i.e. the personal bests)

  \( v_{i,k}(t) \) and \( x_{i,k}(t) \) are **actual velocity / position**

  \( y_{i,k}(t) \) is the **local best position**

  \( \hat{y}_{i,k}(t) \) is the **global best position**
Rules (explained) in the PSO algorithm

How to calculate the position of the particle (already initialized with random values)

Please, consider \{w,c1,c2\} as constants and \{r1,r2\} as values sampled from U(0,1)

• 1\textsuperscript{st} calculate new velocity of the particle
\[ v_{i,k}(t+1) = w * v_{i,k}(t) + c_1 * r_{1,k}(t) * (y_{i,k}(t) - x_{i,k}(t)) + c_2 * r_{2,k}(t) * (\hat{y}_{i,k}(t) - x_{i,k}(t)) \]

  \[ \begin{align*} \text{inertia} & \quad \text{cognitive component} & \quad \text{social component} \end{align*} \]

• 2\textsuperscript{nd} calculate the new position of the particle
\[ x_i(t+1) = x_i(t) + v_{i,k}(t+1) \]
Summarizing and going further!

- The algorithm still needs a K value.

- The population-based search of the PSO algorithm reduces the effect that initial conditions has, as opposed to the K-Means algorithm the search starts from multiple positions in parallel.

- K-means algorithm tends to converge faster (after less evaluations) than the PSO, but usually with a less accurate clustering [4].

- The performance of PSO can further be improved by seeding the initial swarm with the result of the K-Means algorithm (used as one of the particles, while the rest of the swarm is initialized randomly). This is know as Hybrid PSO and K-Means Clustering Algorithm [1].
Rules *(explained)* in the PSO algorithm

- **Initialization** with Random Poses (PSO) + K-Means
- **Evaluate Fitness**
- **Compute Distances**
- **Assign inputs to Clusters**
- **Update Cluster Centroids**
- **Update Local Best and Global Best**
A static example

Resulting clustering with only k-means

Resulting clustering using PSO with k-means initialization.

Look at the blinking circle!
A dynamic example
References


