mean shift聚类算法的MATLAB程序

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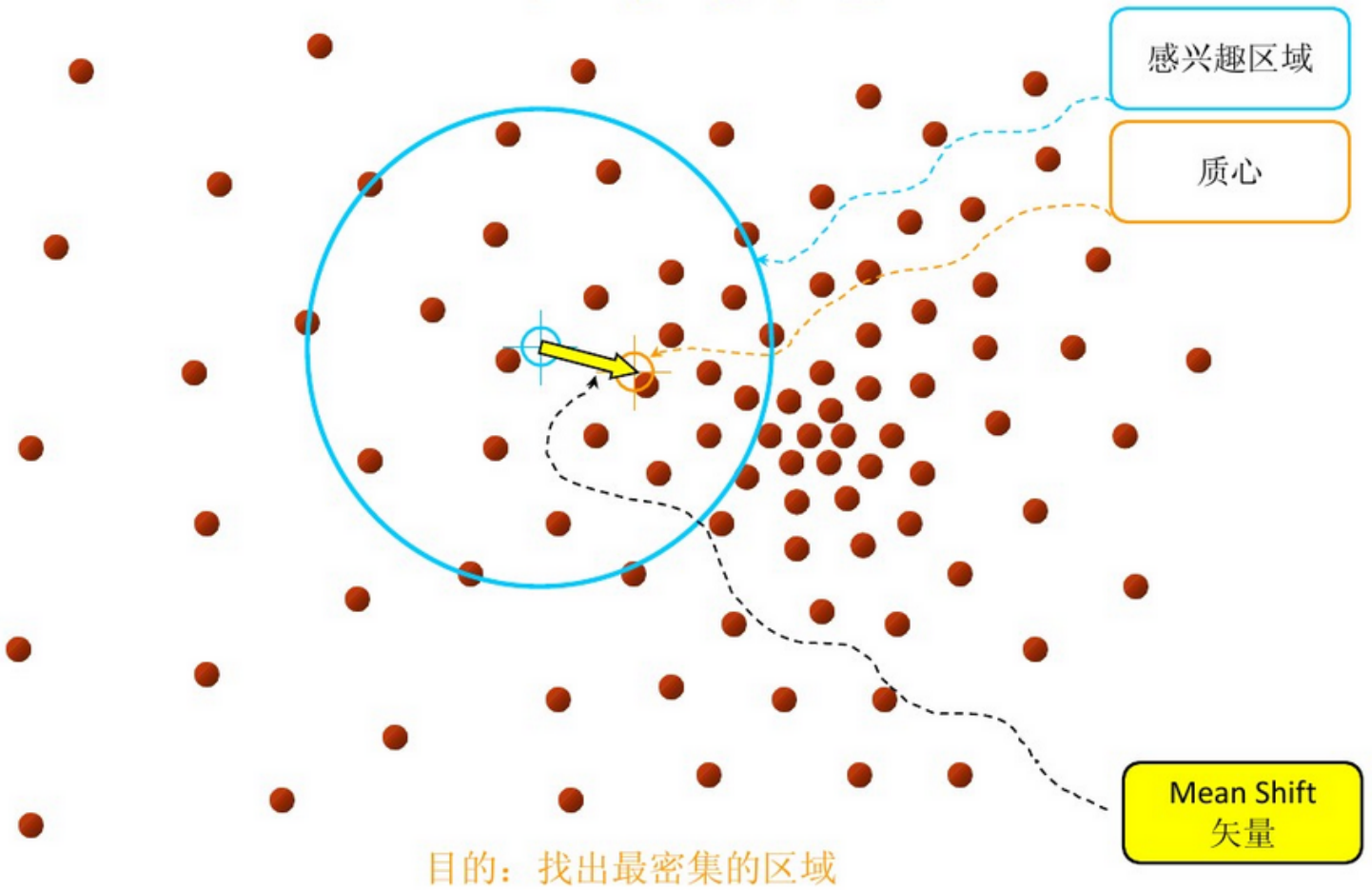
1. mean shift 简介

mean shift, 写的更符合国人的习惯，应该是mean of shift，也就是平均偏移量，或者**偏移均值向量**。在明确了含义之后，就可以开始如下的具体讲解了。



1). 基本形式

$$M_h(x) = \frac{1}{k}\sum_{x_i \in S_h}(x_i - x)$$

其中 $x_i \in \mathbb{R}^d$ 为 n 个样本点，$i = 1, 2, \cdots, n$，S_h 为以 x 为中心的半径为 h 的高维球体，表示有效区域，其中包含 k 个样本点。其变形如下：

$$M_h(x) = \frac{1}{k}\sum_{x_i \in S_h} x_i - x$$

$$\hat{x} = x + M_h(x) = \frac{1}{k}\sum_{x_i \in S_h} x_i$$

由此可以可知，$M_h(x)$ 作为x的偏移均值向量，可用来对 x 进行更新，但这种更新有什么意义呢？通过简单的二维样本模拟，可以发现其倾向于向有效区域中样本密度高（即**概率密度大**）的地方移动。

2). 改进形式

基本形式中隐含了在有效区域中对所有的样本点一视同仁的假设，但这通常是不成立，最常见的就是随着距离的增加，作用就越小，因此，就有了如下的改进形式：

$$M_h(x) = \frac{\sum_{i=1}^{n} G(||\frac{x_i - x}{h}||^2) w(x_i)(x_i - x)}{\sum_{i=1}^{n} G(||\frac{x_i - x}{h}||^2) w(x_i)}$$

其中 $G(||\frac{x_i - x}{h}||^2)$ 为核函数，h 表示带宽（严格来讲因为带宽矩阵，为**对角矩阵**，但通常对角元素取相等，故可表示为标量），$w(x_i)$ 为样本权重。

由此可对**基本形式**进行更为合理的表示，采用均匀核函数，从而达到统一表示：

$$M_h(x) = \frac{\sum_{i=1}^{n} G(||\frac{x_i - x}{h}||^2)(x_i - x)}{\sum_{i=1}^{n} G(||\frac{x_i - x}{h}||^2)}$$

$$G(||\frac{x_i - x}{h}||^2) = \begin{cases} 1, & ||\frac{x_i - x}{h}||^2 <= 1 \\ 0, & else \end{cases}$$

2. mean shift 解释

1)．数学推导

概率密度估计中，常用的方法有直方图估计、K近邻估计、核函数估计，其中核函数估计的表示如下：

$$f(x)=\frac{\sum_{i=1}^{n}K(||\frac{x_i-x}{h}||^2)w(x_i)}{h^d\sum_{i=1}^{n}w(x_i)}$$

其中 $K(||\frac{x_i-x}{h}||^2)$ 同样表示核函数。对概率密度函数 $f(x)$ 求导如下：

$$f(x)=\frac{2\sum_{i=1}^{n}K^{'}(||\frac{x_i-x}{h}||^2)w(x_i)(x-x_i)}{h^{d+2}\sum_{i=1}^{n}w(x_i)}$$

令 $G(||\frac{x_i-x}{h}||^2)=-K^{'}(||\frac{x_i-x}{h}||^2)$,其亦是核函数，进一步分解，有如下表示：

$$\bigtriangledown f(x)=\frac{2}{h^2}\left[\frac{\sum_{i=1}^{n}G(||\frac{x_i-x}{h}||^2)w(x_i)}{h^d\sum_{i=1}^{n}w(x_i)}\right]\left[\frac{\sum_{i=1}^{n}G(||\frac{x_i-x}{h}||^2)w(x_i)(x_i-x)}{G(||\frac{x_i-x}{h}||^2)w(x_i)}\right]$$

可以看出，其中第二项也是一种概率密度的核函数估计，将其表示为 $f_g(x)$ ，第三项则为上文中的mean shift的改进形式，因此，可以改写为：

$$\bigtriangledown f(x)=\frac{2}{h^2}f_g(x)M_h(x)$$

接下来是两种解释，首先，求解概率密度局部极大值，令 $\bigtriangledown f(x)=0$ ，由于 $f_g(x)>0$ ，故有：

$$x^*=\frac{\sum_{i=1}^{n}G(||\frac{x_i-x}{h}||^2)w(x_i)x_i}{G(||\frac{x_i-x}{h}||^2)w(x_i)}=x+M_h(x)$$

这表示mean shift的本质是在求解概率密度局部极大值，即偏移均值向量让目标点始终向概率密度极大点处移动。**但当数据量非常大时，一次遍历所有样本点显然不合适，故常选取目标点 x 附近的一个区域，进行贪心迭代，逐步收敛于概率密度极大值处；另一种更合理的解释是，通过在核函数 $G()$ 中融合进一个均匀核函数来表示选取的有效区域，然后迭代直至收敛。**

再者，从梯度上升的优化角度来讲，有如下表示：

$$M_h(x) = \frac{1}{\frac{2}{h^2} f_g(x)} \bigtriangledown f(x)$$

$$\hat{x} = x + M_h(x) = x + \frac{1}{\frac{2}{h^2} f_g(x)} \bigtriangledown f(x)$$

即偏移均值向量的作用等价于以概率密度为目标的**具有自适应步长的梯度上升优化**，其在概率密度较小的位置步长较大，当逼近局部极大点时，概率密度较大，因此步长较小，符合梯度优化中步长变化的需要。

由此，便对mean shift的含义及其合理性进行了解释，也就不难理解为何mean shift具有强大的效果及适用性了。

2). 泛化拓展

进一步拓展，虽然一般形式的mean shift是由概率密度的核函数估计推导出来的，其核心是核函数，但由于其具有归一化表示的性质，因此，理论上可以泛化为如下表示形式：

$$M_h(x) = \frac{\sum_{i=1}^{n} h(x_i, x)(x_i - x)}{\sum_{i=1}^{n} h(x_i, x)}$$

其中 $h(x_i, x)$确定偏移向量 $x_i - x$ 的整体权重，可以任意选取，但必然需要具有一定的意义。显然偏移均值向量会倾向于权重较大的样本点，因此，从概率密度最大化的角度来看，$h()$ 可以是 x_i 处概率密度的一种表示。

3. mean shift MATLAB程序

testMeanShift.m

```
clear
clc
profile on

bandwidth = 1;
%% 加载数据
```

```
data_load=dlmread('gauss_data.txt');
[~,dim]=size(data_load);
data=data_load(:,1:dim-1);
x=data';
%% 聚类
tic
[clustCent,point2cluster,clustMembsCell] = MeanShiftCluster(x,bandwidth);
% clustCent：聚类中心 D*K, point2cluster：聚类结果 类标签, 1*N
toc
%% 作图
numClust = length(clustMembsCell);
figure(2),clf,hold on
cVec = 'bgrcmykbgrcmykbgrcmykbgrcmyk';%, cVec = [cVec cVec];
for k = 1:min(numClust,length(cVec))
    myMembers = clustMembsCell{k};
    myClustCen = clustCent(:,k);
    plot(x(1,myMembers),x(2,myMembers),[cVec(k) '.'])
    plot(myClustCen(1),myClustCen(2),'o','MarkerEdgeColor','k','MarkerFaceColor',cVec(k), 'MarkerSize',10)
end
title(['no shifting, numClust:' int2str(numClust)])
```

MeanShiftCluster.m

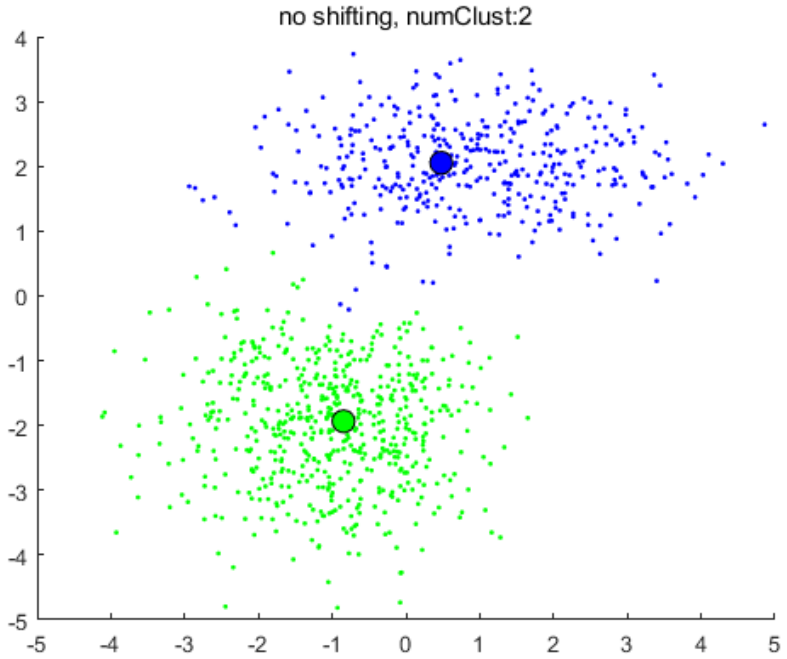
```
function [clustCent,data2cluster,cluster2dataCell] = MeanShiftCluster(dataPts,bandWidth,plotFlag)
%perform MeanShift Clustering of data using a flat kernel
%
% ---INPUT---
% dataPts           - input data, (numDim x numPts)
% bandWidth         - is bandwidth parameter (scalar)
% plotFlag          - display output if 2 or 3 D    (logical)
% ---OUTPUT---
% clustCent         - is locations of cluster centers (numDim x numClust)
% data2cluster      - for every data point which cluster it belongs to (numPts)
% cluster2dataCell  - for every cluster which points are in it (numClust)
%
% Bryan Feldman 02/24/06
% MeanShift first appears in
% K. Funkunaga and L.D. Hosteler, "The Estimation of the Gradient of a
% Density Function, with Applications in Pattern Recognition"


%*** Check input ****
if nargin < 2
    error('no bandwidth specified')
end

if nargin < 3
    plotFlag = true;
    plotFlag = false;
end

%**** Initialize stuff ***
[numDim,numPts] = size(dataPts);
numClust        = 0;
bandSq          = bandWidth^2;
```

```
initPtInds      = 1:numPts;
maxPos          = max(dataPts,[],2);                %biggest size in each dimension
minPos          = min(dataPts,[],2);                %smallest size in each dimension
boundBox        = maxPos-minPos;                    %bounding box size
sizeSpace       = norm(boundBox);                   %indicator of size of data space
stopThresh      = 1e-3*bandWidth;                   %when mean has converged
clustCent       = [];                               %center of clust
beenVisitedFlag = zeros(1,numPts);                  %track if a points been seen already
numInitPts      = numPts;                           %number of points to posibaly use as initilization points
clusterVotes    = zeros(1,numPts);                  %used to resolve conflicts on cluster membership


while numInitPts

    tempInd         = ceil( (numInitPts-1e-6)*rand);        %pick a random seed point
    stInd           = initPtInds(tempInd);                  %use this point as start of mean
    myMean          = dataPts(:,stInd);                     % intilize mean to this points location
    myMembers       = [];                                   % points that will get added to this cluster
    thisClusterVotes    = zeros(1,numPts);                  %used to resolve conflicts on cluster membership

    while 1     %loop untill convergence

        sqDistToAll = sum((repmat(myMean,1,numPts) - dataPts).^2);    %dist squared from mean to all points still active
        inInds      = find(sqDistToAll < bandSq);                     %points within bandWidth
        thisClusterVotes(inInds) = thisClusterVotes(inInds)+1;        %add a vote for all the in points belonging to this cluster


        myOldMean   = myMean;                                   %save the old mean
        myMean      = mean(dataPts(:,inInds),2);                %compute the new mean
        myMembers   = [myMembers inInds];                       %add any point within bandWidth to the cluster
        beenVisitedFlag(myMembers) = 1;                         %mark that these points have been visited

        %*** plot stuff ****
        if plotFlag
            figure(1),clf,hold on
            if numDim == 2
                plot(dataPts(1,:),dataPts(2,:),'.')
                plot(dataPts(1,myMembers),dataPts(2,myMembers),'ys')
                plot(myMean(1),myMean(2),'go')
                plot(myOldMean(1),myOldMean(2),'rd')
                pause
            end
        end

        %**** if mean doesn't move much stop this cluster ***
        if norm(myMean-myOldMean) < stopThresh

            %check for merge posibilities
            mergeWith = 0;
            for cN = 1:numClust
                distToOther = norm(myMean-clustCent(:,cN));     %distance from posible new clust max to old clust max
                if distToOther < bandWidth/2                    %if its within bandwidth/2 merge new and old
                    mergeWith = cN;
                    break;
                end
            end
```

```
            if mergeWith > 0    % something to merge
                clustCent(:,mergeWith)       = 0.5*(myMean+clustCent(:,mergeWith));             %record the max as the mean of the two merged (I know biased twoards new ones)
                %clustMembsCell{mergeWith}    = unique([clustMembsCell{mergeWith} myMembers]);   %record which points inside
                clusterVotes(mergeWith,:)    = clusterVotes(mergeWith,:) + thisClusterVotes;     %add these votes to the merged cluster
            else    %its a new cluster
                numClust                    = numClust+1;                    %increment clusters
                clustCent(:,numClust)       = myMean;                        %record the mean
                %clustMembsCell{numClust}    = myMembers;                     %store my members
                clusterVotes(numClust,:)    = thisClusterVotes;
            end

            break;
        end

    end


    initPtInds      = find(beenVisitedFlag == 0);           %we can initialize with any of the points not yet visited
    numInitPts      = length(initPtInds);                   %number of active points in set

end

[val,data2cluster] = max(clusterVotes,[],1);                %a point belongs to the cluster with the most votes

%*** If they want the cluster2data cell find it for them
if nargout > 2
    cluster2dataCell = cell(numClust,1);
    for cN = 1:numClust
        myMembers = find(data2cluster == cN);
        cluster2dataCell{cN} = myMembers;
    end
end
```

数据见：MATLAB中"fitgmdist"的用法及其GMM聚类算法，保存为gauss_data.txt文件，数据最后一列是类标签。

4. 结果



注意：聚类结果与核函数中的参数带宽bandwidth有很大关系，视具体数据而定。

5. 参考文献

[1] 均值偏移（mean shift）？

[2] Mean Shift Clustering

[3] 简单易学的机器学习算法——Mean Shift聚类算法