MATLAB中“fitgmdist”的用法及其GMM聚类算法

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高斯混合模型的基本原理：聚类——GMM，MATLAB官方文档中有关于fitgmdist的介绍：fitgmdist。我之前写过有关GMM聚类的算法：GMM算法的matlab程序。这篇文章主要应用MATLAB自带的函数来进行聚类。

1．fitgmdist函数介绍

fitgmdist的使用形式：gmm = fitgmdist(X,k,Name,Value)

输入

‘RegularizationValue’, 0。（取值：0， 0.1， 0.01,....，正则化系数，防止协方差奇异）

'CovarianceType', 'full'。（取值： 'full'，协方差矩阵是非对角阵，'diagonal'，协方差矩阵为对角阵）

'Start', 'plus'。 （取值：'randSample'，随机初始化，'plus'，k-means++初始化，'S'，自定义初始化），其中S = struct('mu',init_Mu,'Sigma',init_Sigma,'ComponentProportion',init_Components);

'Options'，statset('Display', 'final', 'MaxIter', MaxIter, 'TolFun', TolFun)。 （'Display'有三个取值：'final' 显示最终的输出结果、'iter' 显示每次迭代的结果、'off' 不显示优化参数信息；'MaxIter'：默认100，最大迭代次数；'TolFun'：默认1e-6，目标函数的终止误差）

输出

gmm.mu：更新完后的聚类中心（均值）

gmm.Sigma：更新完后的协方差矩阵

gmm.ComponentProportion：更新完后的混合比例

gmm.NegativeLogLikelihood：更新完后的负对数似然函数

gmm.NumIterations：实际迭代次数

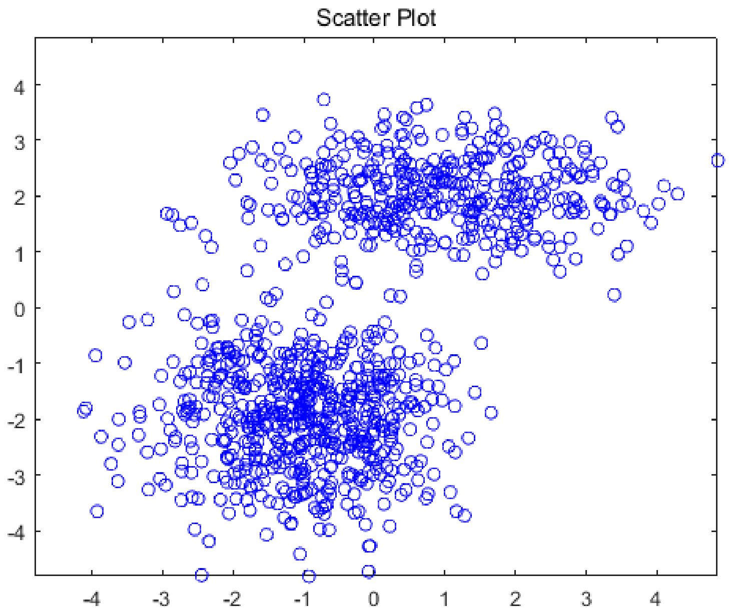
gmm.BIC：贝叶斯信息准则，用于模型选择

更多参数，请在命令行输入properties(gmm)

2．高斯混合模型聚类实例

generate.m

```
function data=generate()
%生成数据
mu1 = [1 2];
Sigma1 = [2 0; 0 0.5];
mu2 = [-1 -2];
Sigma2 = [1 0;0 1];
data = [mvnrnd(mu1,Sigma1,400), ones(400,1);mvnrnd(mu2,Sigma2,600), 2*ones(600,1)];
X=[data(:, 1), data(:, 2)];
figure(1)
plot(X(:,1), X(:,2),'bo')
title('Scatter Plot')
xlim([min(X(:)) max(X(:))]) % Make axes have the same scale
ylim([min(X(:)) max(X(:))])
```



具体数据

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```

GMM_main.m

```
function [accuracy,NumIterations]=GMM_main(data, K)
%主函数
[~, data_dim]=size(data);
X=data(:, 1:data_dim-1);  %数据
real_label=data(:, data_dim);
[label, ~, NumIterations]=Matlab_gmm_2(X, K);
accuracy=succeed(real_label,K,label);
```

Matlab_gmm.m

```
function [label, NegativeLogLikelihood, NumIterations]=Matlab_gmm(X, K)
%协方差矩阵为对角阵，数据独立同分布
[X_num,X_dim]=size(X);
para_sigma_inv=zeros(X_dim, X_dim, K);
N_pdf=zeros(X_num, K);  %单高斯分布的概率密度函数
RegularizationValue=0.001;   %正则化系数，协方差矩阵求逆
MaxIter=100;   %最大迭代次数
TolFun=1e-8;   %终止条件
% 自己设置初始化参数
% init_Mu = [1 1; 2 2];
% init_Sigma(:,:,1) = [1 1; 1 2];
% init_Sigma(:,:,2) = 2*[1 1; 1 2];
% init_Components = [1/2,1/2];
% S = struct('mu',init_Mu,'Sigma',init_Sigma,'ComponentProportion',init_Components);
% gmm=fitgmdist(X, K, 'RegularizationValue', RegularizationValue, 'CovarianceType', 'diagonal', 'Start', 'S', 'Options', statset('Display', 'final', 'MaxIter', MaxIter, 'TolFun', TolFun));
gmm=fitgmdist(X, K, 'RegularizationValue', RegularizationValue, 'CovarianceType', 'diagonal', 'Start', 'plus', 'Options', statset('Display', 'final', 'MaxIter', MaxIter, 'TolFun', TolFun));
```

```
NegativeLogLikelihood=gmm.NegativeLogLikelihood;
NumIterations=gmm.NumIterations;  %迭代次数
mu=gmm.mu;  %均值
Sigma=gmm.Sigma;   %协方差矩阵
ComponentProportion=gmm.ComponentProportion;  %混合比例
for k=1:K
    sigma_inv=1./Sigma(:,:,k);  %sigma的逆矩阵,(X_dim, X_dim)的矩阵
    para_sigma_inv(:, :, k)=diag(sigma_inv);  %sigma^(-1)
end
for k=1:K
    coefficient=(2*pi)^(-X_dim/2)*sqrt(det(para_sigma_inv(:, :, k)));  %高斯分布的概率密度函数e左边的系数
    X_miu=X-repmat(mu(k,:), X_num, 1);  %X-miu: (X_num, X_dim)的矩阵
    exp_up=sum((X_miu*para_sigma_inv(:, :, k)).*X_miu,2);  %指数的幂, (X-miu)'*sigma^(-1)*(X-miu)
    N_pdf(:,k)=coefficient*exp(-0.5*exp_up);
end
responsivity=N_pdf.*repmat(ComponentProportion,X_num,1);  %响应度responsivity的分子, (X_num,K)的矩阵
responsivity=responsivity./repmat(sum(responsivity,2),1,K);  %responsivity:在当前模型下第n个观测数据来自第k个分模型的概率,即分模型k对观测数据Xn的响应度
%聚类
[~,label]=max(responsivity,[],2);
figure(2)
scatter(X(:,1),X(:,2),10,'.') % Scatter plot with points of size 10
hold on
gmPDF = @(x,y)reshape(pdf(gmm,[x(:) y(:)]),size(x));
fcontour(gmPDF,[-6 6])
```

Matlab_gmm_2.m

```
function [label, NegativeLogLikelihood, NumIterations]=Matlab_gmm_2(X, K)
%协方差矩阵为非对角阵,数据不独立
[X_num,X_dim]=size(X);
N_pdf=zeros(X_num, K);  %单高斯分布的概率密度函数
RegularizationValue=0.001;   %正则化系数,协方差矩阵求逆
MaxIter=100;   %最大迭代次数
TolFun=1e-8;   %终止条件
% 自己设置初始化参数
% init_Mu = [1 1; 2 2];
% init_Sigma(:,:,1) = [1 1; 1 2];
% init_Sigma(:,:,2) = 2*[1 1; 1 2];
% init_Components = [1/2,1/2];
% S = struct('mu',init_Mu,'Sigma',init_Sigma,'ComponentProportion',init_Components);
% gmm=fitgmdist(X, K, 'RegularizationValue', RegularizationValue, 'CovarianceType', 'diagonal', 'Start', 'S', 'Options', statset('Display', 'final', 'MaxIter', MaxIter, 'TolFun', TolFun));
gmm=fitgmdist(X, K, 'RegularizationValue', RegularizationValue, 'CovarianceType', 'full', 'Start', 'plus', 'Options', statset('Display', 'final', 'MaxIter', MaxIter, 'TolFun', TolFun));
NegativeLogLikelihood=gmm.NegativeLogLikelihood;
NumIterations=gmm.NumIterations;  %迭代次数
mu=gmm.mu;  %均值
Sigma=gmm.Sigma;   %协方差矩阵
ComponentProportion=gmm.ComponentProportion;  %混合比例
for k=1:K
    X_miu=X-repmat(mu(k,:), X_num, 1);  %X-miu: (X_num, X_dim)的矩阵
    sigma_inv=inv(Sigma(:,:,k));  %sigma的逆矩阵,(X_dim, X_dim)的矩阵
    exp_up=sum((X_miu*sigma_inv).*X_miu,2);  %指数的幂, (X-miu)'*sigma^(-1)*(X-miu)
    coefficient=(2*pi)^(-X_dim/2)*sqrt(det(sigma_inv));  %高斯分布的概率密度函数e左边的系数
    N_pdf(:,k)=coefficient*exp(-0.5*exp_up);
end
responsivity=N_pdf.*repmat(ComponentProportion,X_num,1);  %响应度responsivity的分子, (X_num,K)的矩阵
responsivity=responsivity./repmat(sum(responsivity,2),1,K);  %responsivity:在当前模型下第n个观测数据来自第k个分模型的概率,即分模型k对观测数据Xn的响应度
%聚类
[~,label]=max(responsivity,[],2);
figure(2)
```

```
scatter(X(:,1),X(:,2),10,'.') % Scatter plot with points of size 10
hold on
gmPDF = @(x,y)reshape(pdf(gmm,[x(:) y(:)]),size(x));
fcontour(gmPDF,[-6 6])
```

succeed.m

```
function accuracy=succeed(real_label,K,id)
%输入K：聚的类，id：训练后的聚类结果，N*1的矩阵
N=size(id,1);   %样本个数
p=perms(1:K);   %全排列矩阵
p_col=size(p,1);   %全排列的行数
new_label=zeros(N,p_col);   %聚类结果的所有可能取值，N*p_col
num=zeros(1,p_col);  %与真实聚类结果一样的个数
%将训练结果全排列为N*p_col的矩阵，每一列为一种可能性
for i=1:N
    for j=1:p_col
        for k=1:K
            if id(i)==k
                new_label(i,j)=p(j,k);  %iris数据库，1 2 3
            end
        end
    end
end
%与真实结果比对，计算精确度
for j=1:p_col
    for i=1:N
        if new_label(i,j)==real_label(i)
                num(j)=num(j)+1;
        end
    end
end
accuracy=max(num)/N;
```

结果

以第二种情况为例，数据不独立，协方差矩阵不是只在对角线上有元素。

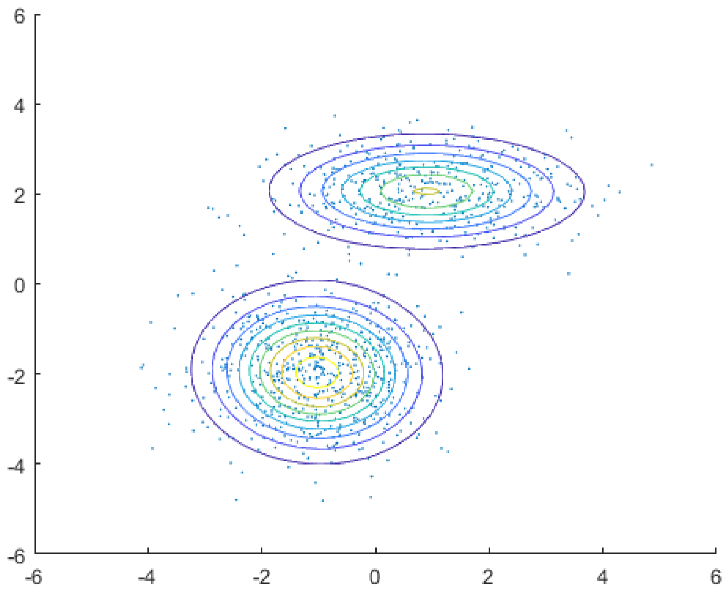
```
>> [accuracy,NumIterations]=GMM_main(data, 2)
32 iterations, log-likelihood = -3449.42

accuracy =

   0.995000000000000


NumIterations =

    32
```


6
4
2
0
-2
-4
-6
-6
-4
-2
0
2
4
6