机器学习算法之KMeans聚类算法

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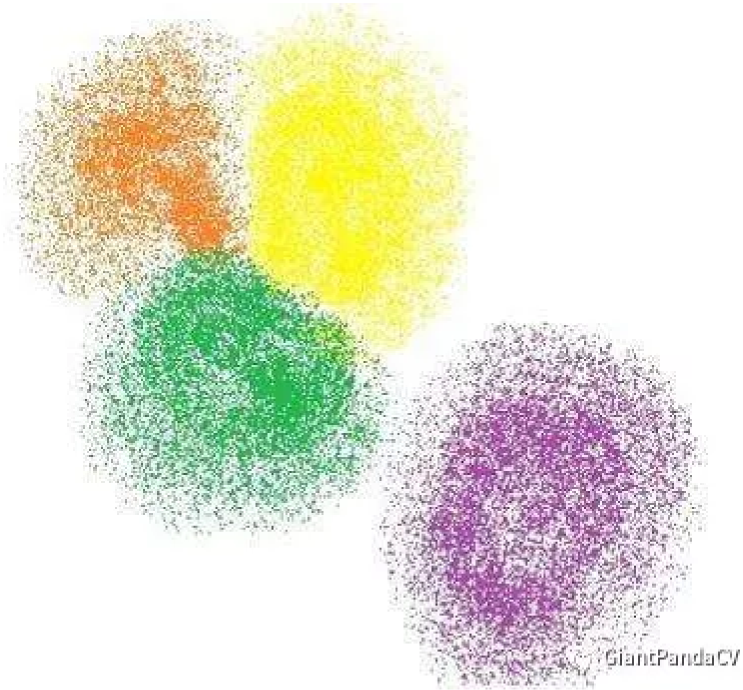
算法原理

聚类指的是把集合，分组成多个类，每个类中的对象都是彼此相似的。K-means是聚类中最常用的方法之一，它是基于点与点距离的相似度来计算最佳类别归属。

在使用该方法前，要注意（1）对数据异常值的处理；（2）对数据标准化处理（x-min(x))/(max(x)-min(x)）；（3）每一个类别的数量要大体均等；（4）不同类别间的特质值应该差异较大。下图展示了一个聚类算法的结果：



算法流程

（1）选择k个初始聚类中心
（2）计算每个对象与这k个中心各自的距离，按照最小距离原则分配到最邻近聚类
（3）使用每个聚类中的样本均值作为新的聚类中心
（4）重复步骤（2）和（3）直到聚类中心不再变化
（5）结束，得到k个聚类

算法的作用

聚类算法可以将数据中相似度比较大的数据聚集在一起，并且此算法是无监督算法，没有任何标注成本。且以KMean聚类算法为基础，衍生了很多其他种类的聚类算法如密度聚类，谱聚类等。在商业上，聚类可以帮助市场分析人员从消费者数据库中区分出不同的消费群体来，并且概括出每一类消费者的消费模式或者说习惯。同时聚类算法在数据挖掘对于数据预处理上也发挥着重要作用。这里只是简单介绍和实现了KMean聚类算法，详细了解推荐《周志华机器学习》书籍。

代码实现

```
#coding=utf-8
from collections import Counter
from copy import deepcopy
from time import time
from random import randint, seed, random

# 统计程序运行时间函数
# fn代表运行的函数
def run_time(fn):
    def fun():
        start = time()
        fn()
        ret = time() - start
        if ret < 1e-6:
            unit = "ns"
            ret *= 1e9
        elif ret < 1e-3:
            unit = "us"
            ret *= 1e6
        elif ret < 1:
            unit = "ms"
            ret *= 1e3
        else:
            unit = "s"
        print("Total run time is %.1f %s\n" % (ret, unit))
    return fun()

def load_data():
    f = open("boston/breast_cancer.csv")
    X = []
    y = []
    for line in f:
        line = line[:-1].split(',')
        xi = [float(s) for s in line[:-1]]
        yi = line[-1]
        if '.' in yi:
            yi = float(yi)
```

```python
        else:
            yi = int(yi)
        X.append(xi)
        y.append(yi)
    f.close()
    return X, y

# 将数据归一化到[0, 1]范围
def min_max_scale(X):
    m = len(X[0])
    x_max = [-float('inf') for _ in range(m)]
    x_min = [float('inf') for _ in range(m)]
    for row in X:
        x_max = [max(a, b) for a, b in zip(x_max, row)]
        x_min = [min(a, b) for a, b in zip(x_min, row)]

    ret = []
    for row in X:
        tmp = [(x - b) / (a - b) for a, b, x in zip(x_max, x_min, row)]
        ret.append(tmp)
    return ret

def get_euclidean_distance(arr1, arr2):
    return sum((x1 - x2) ** 2 for x1, x2 in zip(arr1, arr2)) ** 0.5

def get_cosine_distance(arr1, arr2):
    numerator = sum(x1 * x2 for x1, x2 in zip(arr1, arr2))
    denominator = (sum(x1 ** 2 for x1 in arr1) *
                   sum(x2 ** 2 for x2 in arr2)) ** 0.5
    return numerator / denominator


class KMeans(object):
    # k 簇的个数
    # n_features 特征的个数
    # clister_centers 聚类中心
    # distance_fn 距离计算函数
    # cluster_samples_cnt 每个簇里面的样本数
    def __init__(self):
        self.k = None
```

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        self.n_features = None
        self.cluster_centers = None
        self.distance_fn = None
        self.cluster_samples_cnt = None

    # 二分，查找有序列表里面大于目标值的第一个值
    def bin_search(self, target, nums):
        low = 0
        high = len(nums) - 1
        assert nums[low] <= target < nums[high], "Cannot find target!"
        while 1:
            mid = (low + high) // 2
            if mid == 0 or target >= nums[mid]:
                low = mid + 1
            elif target < nums[mid - 1]:
                high = mid - 1
            else:
                break
        return mid

    # 比较两个向量是否为同一向量
    def cmp_arr(self, arr1, arr2, eps=1e-8):
        return len(arr1) == len(arr2) and \
               all(abs(a- b) < eps for a, b in zip(arr1, arr2))

    # 初始化聚类中心
    def init_cluster_centers(self, X, k, n_features, distance_fn):
        n = len(X)
        centers = [X[randint(0, n-1)]]
        for _ in range(k-1):
            center_pre = centers[-1]
            idxs_dists = ([i, distance_fn(Xi, center_pre)] for i, Xi in enur
            # 对距离进行排序
            idxs_dists = sorted(idxs_dists, key=lambda x: x[1])
            dists = [x[1] for x in idxs_dists]
            tot = sum(dists)
            for i in range(1, n):
                dists[i] /= tot
            for i in range(1, n):
                dists[i] += dists[i-1]
```

```
            # 随机选择一个聚类中心
            while 1:
                num = random()
                # 查找>=num的距离
                dist_idx = self.bin_search(num, dists)
                row_idx = idxs_dists[dist_idx][0]
                center_cur = X[row_idx]
                if not any(self.cmp_arr(center_cur, center) for center in ce
                    break
            centers.append(center_cur)
        return centers


    # 寻找距离Xi最近的聚类中心
    def get_nearest_center(self, Xi, centers, distance_fn):
        return min(((i, distance_fn(Xi, center)) for
                    i, center in enumerate(centers)), key=lambda x: x[1])[0

    # 寻找X最近的聚类中心
    def get_nearest_centers(self, X, distance_fn, centers):
        return [self.get_nearest_center(Xi, centers, distance_fn) for Xi in

    # 获取空的簇
    def get_empty_cluster_idxs(self, cluster_samples_cnt, k):
        clusters = ((i, cluster_samples_cnt[i]) for i in range(k))
        empty_clusters = filter(lambda x: x[1] == 0, clusters)
        return [empty_clusters[0] for empty_cluster in empty_clusters]
    # 在X中找到到所有非空簇中心的最远样本
    def get_furthest_row(self, X, distance_fn, centers, empty_cluster_idxs)
        def f(Xi, centers):
            return sum(distance_fn(Xi, centers) for center in centers)

        non_empty_centers = map(lambda x: x[1], filter(
            lambda x: x[0] not in empty_cluster_idxs, enumerate(centers)))
        return max(map(lambda x: [x, f(x, non_empty_centers)], X), key=lamb

    # 处理空的簇
    def process_empty_clusters(self, X, distance_fn, n_features, centers, em
        for i in empty_cluster_idxs:
            center_cur = self.get_furthest_row(X, distance_fn, centers, emp
```

```
            while any(self._cmp_arr(center_cur, center) for center in center
                center_cur = self.get_furthest_row(X, distance_fn, centers,
                                                    empty_cluster_idxs)
            centers[i] = center_cur
        return centers

    # 重新获取聚类中心
    def get_cluster_centers(self, X, k, n_features, y, cluster_samples_cnt)
        ret = [[0 for _ in range(n_features)] for _ in range(k)]
        for Xi, cetner_num in zip(X, y):
            for j in range(n_features):
                ret[cetner_num][j] += Xi[j] / cluster_samples_cnt[cetner_nur
        return ret

    # 训练
    def fit(self, X, k, fn=None, n_iter=100):
        n_features = len(X[0])
        if fn is None:
            distance_fn = get_euclidean_distance
        else:
            error_msg = "Parameter distance_fn must be eu or cos!"
            assert fn in ("eu", "cos"), error_msg
            if fn == "eu":
                distance_fn = get_euclidean_distance
            if fn == "cos":
                distance_fn = get_cosine_distance

        centers = self.init_cluster_centers(X, k, n_features, distance_fn)
        for i in range(n_iter):
            while 1:
                # 寻找X的最近聚类中心
                y = self.get_nearest_centers(X, distance_fn, centers)
                # 统计每个簇的样本个数
                cluster_samples_cnt = Counter(y)
                # 获取空的簇
                empty_cluster_idxs = self.get_empty_cluster_idxs(cluster_sar
                # 如果有空的簇
                if empty_cluster_idxs:
                    centers = self.process_empty_clusters(centers, empty_clu
                else:
```

```
                    break
                centers_new = self.get_cluster_centers(X, k, n_features, y, clus
                centers = deepcopy(centers_new)
                print("Iteration: %d" % i)
            self.k = k
            self.n_features = n_features
            self.distance_fn = distance_fn
            self.cluster_centers = centers
            self.cluster_samples_cnt = cluster_samples_cnt

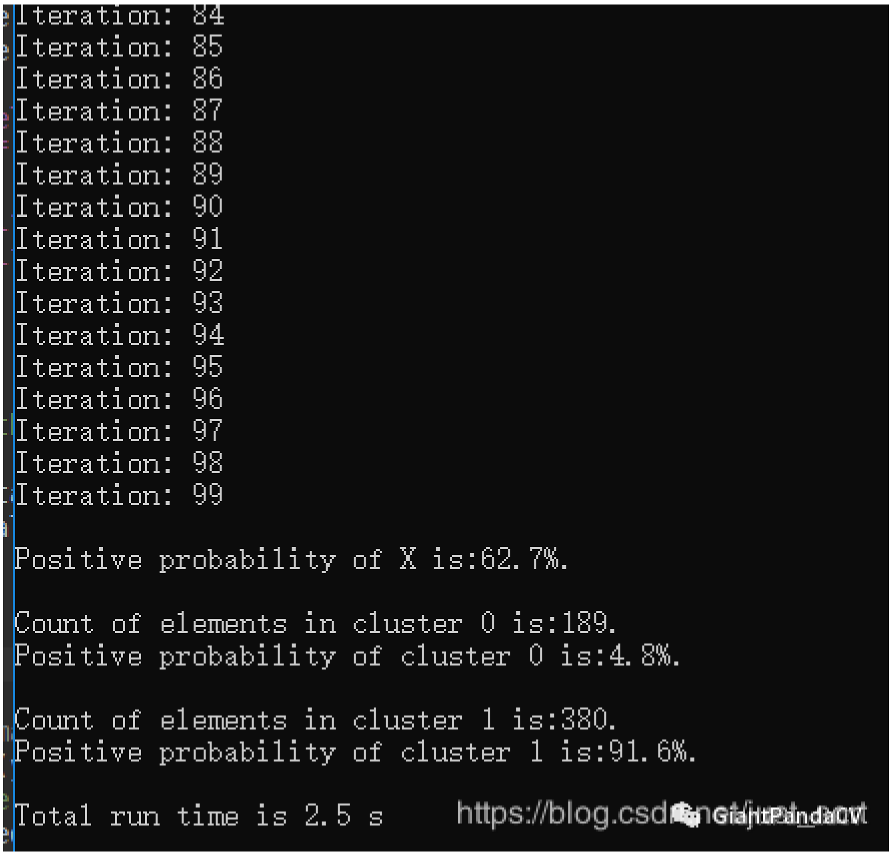
        def _predict(self, Xi):
            return self.get_nearest_center(Xi, self.cluster_centers, self.distar

        def predict(self, X):
            return [self._predict(Xi) for Xi in X]


    @run_time
    def main():
        print("Tesing the performance of Kmeans...")
        # Load data
        X, y = load_data()
        X = min_max_scale(X)
        # Train model
        est = KMeans()
        k = 2
        est.fit(X, k)
        print()
        # Model performance
        prob_pos = sum(y) / len(y)
        print("Positive probability of X is:%.1f%%.\n" % (prob_pos * 100))
        y_hat = est.predict(X)
        cluster_pos_tot_cnt = {i: [0, 0] for i in range(k)}
        for yi_hat, yi in zip(y_hat, y):
            cluster_pos_tot_cnt[yi_hat][0] += yi
            cluster_pos_tot_cnt[yi_hat][1] += 1
        cluster_prob_pos = {k: v[0] / v[1] for k, v in cluster_pos_tot_cnt.items
        for i in range(k):
            tot_cnt = cluster_pos_tot_cnt[i][1]
            prob_pos = cluster_prob_pos[i]
```

```
        print("Count of elements in cluster %d is:%d." %
              (i, tot_cnt))
        print("Positive probability of cluster %d is:%.1f%%.\n" % (i, prob_
```

对肺癌数据集聚类100轮结果



```
Iteration: 84
Iteration: 85
Iteration: 86
Iteration: 87
Iteration: 88
Iteration: 89
Iteration: 90
Iteration: 91
Iteration: 92
Iteration: 93
Iteration: 94
Iteration: 95
Iteration: 96
Iteration: 97
Iteration: 98
Iteration: 99

Positive probability of X is:62.7%.

Count of elements in cluster 0 is:189.
Positive probability of cluster 0 is:4.8%.

Count of elements in cluster 1 is:380.
Positive probability of cluster 1 is:91.6%.

Total run time is 2.5 s
```

可以看到经过100次聚类后，正负样本被大量聚集在了一起，证明了聚类算法的有效性。

源码和数据集获取

https://github.com/BBuf/machine-learning