Lab2 实验报告

牛庆源 PB21111733

part_1 传统机器学习

1. 决策树

1. 根据训练数据构建决策树并在测试集上测试。构建决策树的过程主体是一个递归的过程:
   - 读入数据 → 生成节点 → 判断节点是否可以划分属性 → 选择最优划分 → 生成分支

   递归进行。

   1. 判断部分（出口）： 若为空则赋值 Null； 若样本都属于类别C则标记为C类叶节点。判断结束本次递归结束。
   2. 选择最优划分部分的依据为信息增益，依据实验文档给出的公式计算。
   3. 连续值处理采用二分法离散化。
2. 具体过程:
   1. 计算信息熵:

```
def entropy(y):
    classes, counts = np.unique(y, return_counts=True)
    probabilities = counts / len(y)
    return -np.sum(probabilities * np.log2(probabilities))
```

   2. 计算信息增益（二分法处理连续值）：

```
# 信息增益
    def info_gain(self, X, y, feature, threshold):
        left_idx = X[:, feature] < threshold
        right_idx = X[:, feature] >= threshold
        left_entropy = self.entropy(y[left_idx])
        right_entropy = self.entropy(y[right_idx])
        return self.entropy(y) - np.mean(left_idx) * left_entropy -
np.mean(right_idx) * right_entropy
```

   3. 遍历分割点选择最佳分割:

```python
# 选择最佳分割点
    def best_split(self, X, y):
        best_feature, best_threshold, best_info_gain = None, None, -
np.inf
        n_features = X.shape[1]
        for feature in range(n_features):
            thresholds = np.unique(X[:, feature])
            for threshold in thresholds:
                ig = self.info_gain(X, y, feature, threshold)
                if ig > best_info_gain:
                    best_feature, best_threshold, best_info_gain =
feature, threshold, ig
        return best_feature, best_threshold, best_info_gain
```

④ 构建决策树

```python
# 递归构建决策树
    def build_tree(self, X, y, max_depth, min_samples_leaf):
        if len(y) == 0:
            return {'threshold': None}
        if max_depth == 0 or len(y) < min_samples_leaf:
            return {'threshold': np.argmax(np.bincount(y))}
        feature, threshold, info_gain = self.best_split(X, y)
        # 信息增益为0
        if info_gain == 0:
            return {'threshold':np.argmax(np.bincount(y))}
        left_idx = X[:, feature] < threshold
        right_idx = X[:, feature] >= threshold
        left_tree = self.build_tree(X[left_idx], y[left_idx],
max_depth-1, min_samples_leaf)
        right_tree = self.build_tree(X[right_idx], y[right_idx],
max_depth-1, min_samples_leaf)
        return {'feature': feature,
                'threshold': threshold,
                'left_tree': left_tree,
                'right_tree': right_tree}
```

⑤ 做出预测

```python
def predict(self, X):
        # X: [n_samples_test, n_features],
        # return: y: [n_samples_test, ]
        X = np.array(X)
        y = np.zeros(X.shape[0])

        for i in range(X.shape[0]):
            node = self.tree
            while 'feature' in node:
                if X[i][node['feature']] < node['threshold']:
                    node = node['left_tree']
                else:
                    node = node['right_tree']
            y[i] = node['threshold']
        return y
```

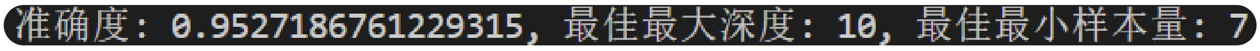
3 调试参数

```
accuracy_init = 0
    for i in range(5, 12):
        max_depth = i
        for j in range(2, 10):
            min_samples_leaf = j
            clf.fit(X_train, y_train, max_depth=max_depth,
min_samples_leaf=min_samples_leaf)
            y_pred = clf.predict(X_test)
            if accuracy(y_test, y_pred) > accuracy_init:
                accuracy_init = accuracy(y_test, y_pred)
                max_depth_best = max_depth
                min_samples_leaf_best = min_samples_leaf

print(f"准确度: {accuracy_init}, 最佳最大深度: {max_depth_best}, 最佳最小样本
量: {min_samples_leaf_best}")
```

最大深度从5到11，最小样本量从2到9。

最大深度为最佳准确率和最佳参数如下:



```
准确度: 0.9527186761229315, 最佳最大深度: 10, 最佳最小样本量: 7
```

2. PCAKMeans

1 PCA

1 核函数:

```python
def get_kernel_function(kernel):
    if kernel == "rbf":
        def rbf_kernel(x, y, gamma=1.0):
            return np.exp(-gamma * np.linalg.norm(x - y) ** 2)
        return rbf_kernel
    # 这里使用线性核
    elif kernel == "linear":
        def linear_kernel(x, y):
            return np.dot(x, y)
        return linear_kernel
    else:
        raise ValueError("Unsupported kernel")
```

2. 主成分分析：

```python
def fit(self, X: np.ndarray):
        # X: [n_samples, n_features]
        n_samples = X.shape[0]
        K = np.zeros((n_samples, n_samples))

        for i in range(n_samples):
            for j in range(n_samples):
                K[i, j] = self.kernel_f(X[i], X[j])

        # 中心化
        one_n = np.ones((n_samples, n_samples)) / n_samples
        K_centered = K - one_n @ K - K @ one_n + one_n @ K @ one_n
        self.K = K_centered

        # Eigenvalue decomposition
        eigenvalues, eigenvectors = np.linalg.eig(K_centered)
        idx = eigenvalues.argsort()[::-1]

        self.eigenvectors = eigenvectors[:, idx[:self.n_components]]
        self.eigenvalues = eigenvalues[idx[:self.n_components]]
```

3. 投影： $x'_j = \frac{1}{\sqrt{\lambda}}[K(x_1, x_j), \ldots, K(x_n, x_j)] \cdot u$

```python
def transform(self, X: np.ndarray):
        # X: [n_samples, n_features]
        self.fit(X)
        X_reduced = (self.K @ self.eigenvectors) /
np.sqrt(self.eigenvalues[:self.n_components])

        return X_reduced
```

2. KMeans
   1. 初始化。
   2. 计算每个点到各个中心的距离，并分配到最近的聚类。

```python
def assign_points(self, points):
        n_samples = points.shape
        self.labels = np.zeros(n_samples, dtpe = int)
        for i in range(n_samples):
            distances = np.linalg.norm(points[i] - self.centers,
axis=1)
            self.labels[i] = np.argmin(distances)
        return self.labels
```

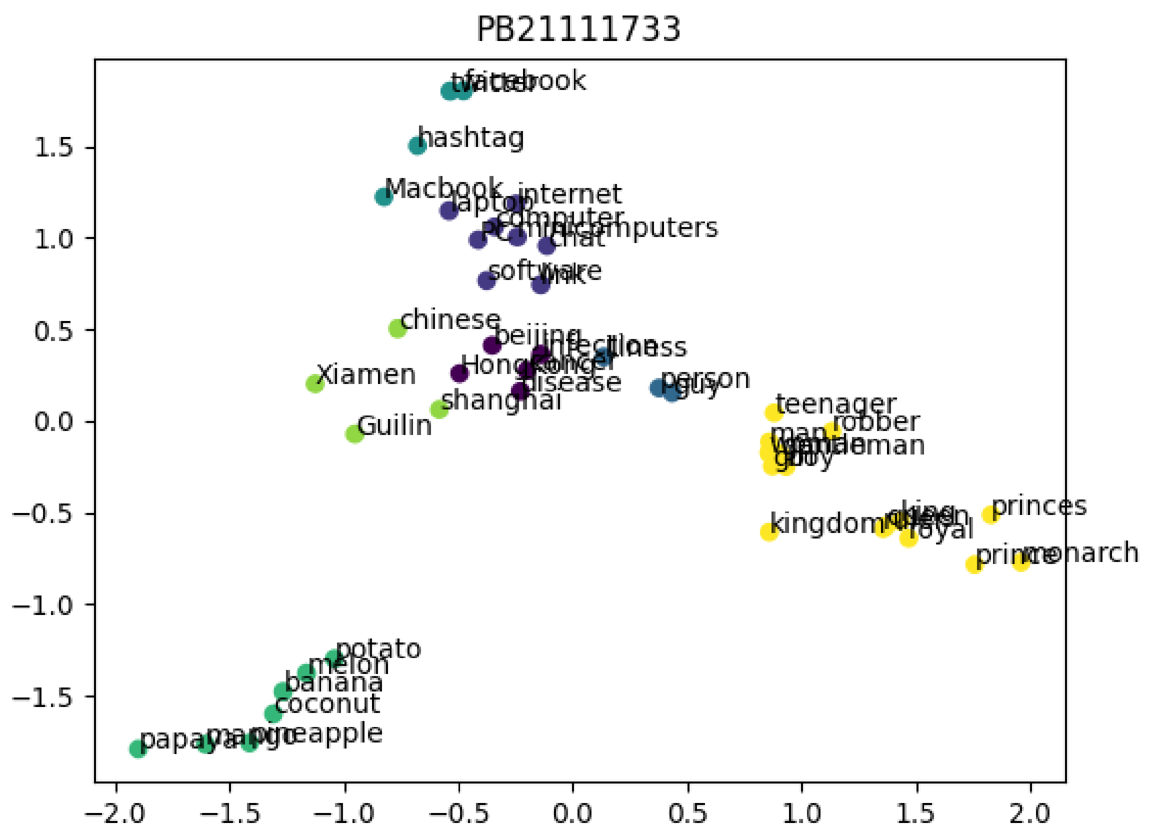
   3. 更新聚类中心。

```python
def update_centers(self, points):
        for i in range(self.k):
            cluster_points = points[self.labels == i]
            if len(cluster_points) > 0:
                self.centers[i] = cluster_points.mean(axis=0)
            else:
                self.centers[i] =
points[np.random.choice(len(points))]
```

   4. KMeans执行。（使用 `allclose` 判断两个数组的元素是否逐一接近）

```python
def fit(self, points):
        self.centers = self.initialize_centers(points)
        for _ in range(self.max_iter):
            previous_centers = self.centers.copy()
            self.labels = self.assign_points(points)
            self.update_centers(points)
            if np.allclose(previous_centers, self.centers):
                break
```

3 测试：分解到2维，使用`linear`核。7个聚类。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