

# kNN分类算法

## 1. 数据集

数据集的散点图,举例. 注意: mglearn,matplotlib的使用.

```
import mglearn
import matplotlib.pyplot as plt

# generate dataset
X,y = mglearn.datasets.make_forge()
# x是一个二维的np数组
print(X[:,0])
# y是一个一维的np数组

# plot dataset
mglearn.discrete_scatter(X[:,0],X[:,1],y)
plt.legend(["Class 0", "Class 1"])
plt.xlabel("x1")
plt.ylabel("x2")
print("X.shape: {}".format(X.shape))
plt.show()
```

```
[ 9.96346605 11.0329545 11.54155807  8.69289001  8.1062269  8.30988863
 11.93027136  9.67284681  8.34810316  8.67494727  9.17748385 10.24028948
  8.68937095  8.92229526  9.49123469  9.25694192  7.99815287  8.18378052
  8.7337095   9.32298256 10.06393839  9.50048972  8.34468785  9.50169345
  9.15072323 11.563957 ]
X.shape: (26, 2)
```

<Figure size 640x480 with 1 Axes>

特征数目: 2 样本数目: 26 类别: 2

kNN分类算法是最简单的机器学习算法. 我们要先自己构建该算法, 这样非常有助于我们理解. 而不是简单地调用已有的库函数.

问题: 对于一个我们从未见过的数据样本, 我们想知道它属于什么类别. (做图, 如上.)

kNN算法从整个训练集里找出离这个新数据样本最近的邻域内的样本.

然后, 该算法做一个关于类别的投票(mode vote), 从而决定新的样本属于哪一类.

因为必须计算新样本到所有训练样本的距离,

kNN的执行速度依赖于类别的数目, 以及样本的数目.

我们可以用任意我们自定义的距离函数,而不必局限于欧几里得距离。

极端一点例子: 0 或1,对那些名义上的特征可用。

理解kNN比较容易,因而它称为数据科学家学习的第一个机器学习算法。

当我们想写一个分类器时,我们可以考虑用kNN算法。

## 2. 求N维空间中两点之间的距离

```
import numpy as np

def distance(p1, p2):
    """返回两点间的距离(欧几里得距离, Euclidean distance)
    这个定义具有普遍性,可用于计算N维空间中的两点的距离。
    """
    return np.sqrt(np.sum(np.power(p1 - p2, 2)))

a = np.array([4,0])
c = np.array([4,3])

print(distance(a,c))

x = np.array([0,0,0,0])
y = np.array([4,3,2,2])

print(distance(x,y))

# 附: 求出OA与OC的夹角.
a = np.array([4,0])
c = np.array([4,3])
o = np.zeros(2)
len_OA = distance(a,o)
len_OC = distance(c,o)
cos_theta = np.sum(a * c) / (len_OA * len_OC)
print(np.arccos(cos_theta))
```

```
3.0
5.744562646538029
0.6435011087932843
```

## 3. 投票函数

# 类似于求词频的函数count\_words(text), 定义如下函数count\_votes(votes)。

```
def count_votes(votes):
    count_dict = {}
    for vote in votes:
```

```

# known word
if vote in count_dict:
    count_dict[vote] += 1
else:
    count_dict[vote] = 1
return count_dict

# 定义一个序列
votes = [1,2,1,3,4,2,2,2,3,3,2,3,3]

# 调用函数,得到字典
vote_count = count_votes(votes)
vote_count

```

```
{1: 2, 2: 5, 3: 5, 4: 1}
```

在上面的例子中,序列votes中,2 出现了5次. 次数最多,频率最高. 问,我们如何把出现频率最高者找到并提取出来呢?

```
max(vote_count.keys())
```

```
4
```

```
max(vote_count.values())
```

```
5
```

```
max_count = max(vote_count.values())
max_count
```

```
5
```

items()方法: 提取出关键字和对应的值.

```
for vote, counts in vote_count.items():
    print(vote, counts)
```

```
1 2
2 5
3 5
4 1
```

一个序列中可能有多个最高频者(胜利者). 所以我们用列表来保存它们,命名为winners.

```
winners = []
max_count = max(vote_count.values())
for vote, counts in vote_count.items():
    if counts == max_count:
        print(vote, counts)
        winners.append(vote)
    print(winners)
```

```
2 5
[2]
3 5
[2, 3]
```

进一步简化函数

```
def majority_vote(votes):
    count_dict = {}

    for vote in votes:
        # 已见过的选项(vote)
        if vote in count_dict:
            count_dict[vote] += 1
        # 未见过的选项
        else:
            count_dict[vote] = 1

    winners = []
    max_count = max(count_dict.values())
    for vote, counts in count_dict.items():
        if counts == max_count:
            winners.append(vote)
    return winners    # 注意缩进

majority_vote(votes)
```

```
[2, 3]
```

进一步修改, 我们只需要从众多的胜利者中选出一个就可以了. 所以我们随机选择一个. 引用random模块, 修改如下:

```
import random

def majority_vote(votes):
    count_dict = {}

    for vote in votes:
        # 已见过的选项(vote)
        if vote in count_dict:
            count_dict[vote] += 1
        # 未见过的选项
        else:
            count_dict[vote] = 1

    winners = []
    max_count = max(count_dict.values())
    for vote, counts in count_dict.items():
        if counts == max_count:
            winners.append(vote)
    return random.choice(winners)

majority_vote(votes)
```

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一个序列(或其他数据结构)中的最高频者, 常称为模式(Mode), 或称众数.

找出一个序列中最高频的元素, 是统计学中的极其常见和基本的操作.

如何找到一个NumPy数组的众数呢?

scipy.stats.mode()可直接实现之. majority\_vote(votes)更简洁的版本如下:

```
import numpy as np
import scipy.stats as ss # 导入scipy.stats(约定)

def majority_vote_simple(votes):
    """
    返回序列中的最高频元素.
    输入: NumPy数组
    """
    mode, count = ss.mstats.mode(votes)
    return mode

votes = [1, 2, 1, 1, 2, 3, 1, 5, 6, 3]
votes = np.array(votes)
```

```
majority_vote_simple(votes)
```

```
array([1.])
```

```
random.choice([2])
```

```
2
```

## 4. 如何找到最近邻居?

### 4.1 什么是"最近邻居"?

前提: 空间, 距离.

操作: 比较距离的大小, 排序.

### 4.2. 找出最近邻居

"求最近邻居算法"之基本思想:

对所有的点:  
    求出其中一点p与其他各点的距离  
对距离排序, 并返回离p点最近的k个点

举例如下:

```
# 先举例:可视化所有的点

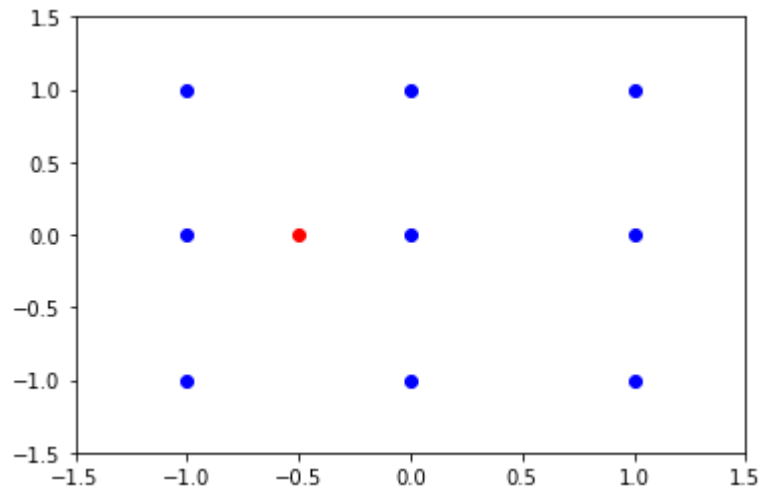
import matplotlib.pyplot as plt

points = np.array([[ -1, -1], [ -1, 0], [ -1, 1], [ 0, -1], [ 0, 0], [ 0, 1], [ 1, -1], [ 1, 0], [ 1, 1]])
p = np.array([ -0.5, 0])

plt.plot(points[:,0], points[:,1], "ob");
plt.plot(p[0],p[1], "or")

# 设置作图范围
plt.axis([ -1.5, 1.5, -1.5, 1.5])
```

```
[-1.5, 1.5, -1.5, 1.5]
```



现在开始写函数.

```
import matplotlib.pyplot as plt

points = np.array([[-1,-1],[-1,0],[-1,1],[0,-1],[0,0],[0,1],[1,-1],[1,0],[1,1]])
p = np.array([-0.5, 0])

distances = np.zeros(points.shape[0])
for i in range(len(distances)):
    distances[i] = distance(points[i],p)

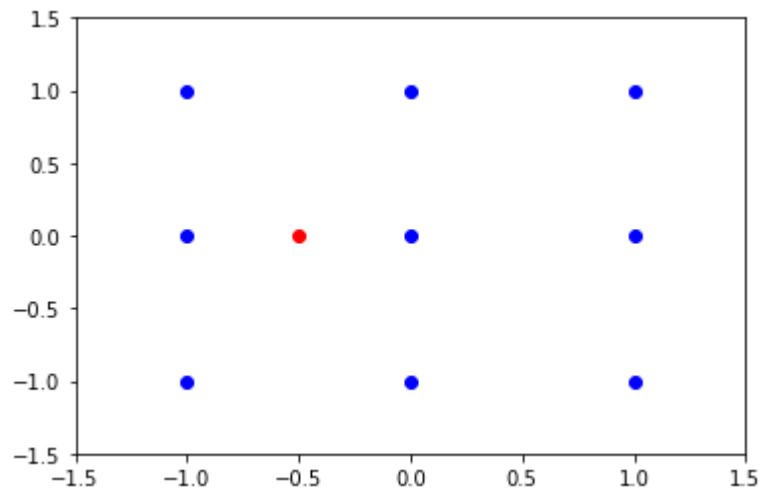
# 打印出points中的点与p点的距离.
print("p点与序列中的点的距离:",distances)

plt.plot(points[:,0], points[:,1], "ob");
plt.plot(p[0],p[1], "or")

# 设置作图范围
plt.axis([-1.5,1.5,-1.5,1.5])
```

```
p点与序列中的点的距离: [1.11803399 0.5      1.11803399 1.11803399 0.5      1.11803399
 1.80277564 1.5       1.80277564]
```

```
[-1.5, 1.5, -1.5, 1.5]
```



如何对这些距离按由小到大顺序做排序? NumPy中有一个这样的函数argsort(). 它返回最小的k个值的index.

```
print(distances)
np.argsort(distances)
```

```
[1.11803399 0.5      1.11803399 1.11803399 0.5      1.11803399
 1.80277564 1.5      1.80277564]
```

```
array([1, 4, 0, 2, 3, 5, 7, 6, 8], dtype=int64)
```

最小的两个距离值是第2个点和第5个点. 距离都为0.5.

```
# 将argsort()之返回值赋给一个索引对象ind.
ind = np.argsort(distances)
# 计算出距离值(由小到大排序):
distances[ind]
```

```
array([0.5      , 0.5      , 1.11803399, 1.11803399, 1.11803399,
       1.11803399, 1.5      , 1.80277564, 1.80277564])
```

如果只想求距离最短的两个值,命令如下:

```
distances[ind[:2]]
```



(9, 2)

现在,我们可以写出求k个最近邻居的函数: find\_nn(p,points,k)

```
def find_nn(p,points, k=3):
    """
    返回(points集合中)距离p点最近的k个点的索引值.
    """
    #points.shape
    distances = np.zeros(points.shape[0])
    for i in range(len(distances)):
        distances[i] = distance(points[i],p)
    ind = np.argsort(distances)
    # 计算出距离值(由小到大排序):
    #return ind[0:k]
    return ind[:k]

#计算最近邻居
k = 3
points = np.array([[ -1, -1], [ -1, 0], [ -1, 1], [ 0, -1], [ 0, 0], [ 0, 1], [ 1, -1], [ 1, 0], [ 1, 1]])
p = np.array([ -0.5, 0])
ind = find_nn(p,points,k)
print("最近的{}个点的索引:\n{}".format(len(ind),ind))
print("最近的{}个点的坐标:\n{}".format(len(ind),points[ind]))

#作图
plt.plot(points[:,0],points[:,1], "bo")
plt.plot(p[0],p[1], "ro")
```

最近的3个点的索引:

[1 4 0]

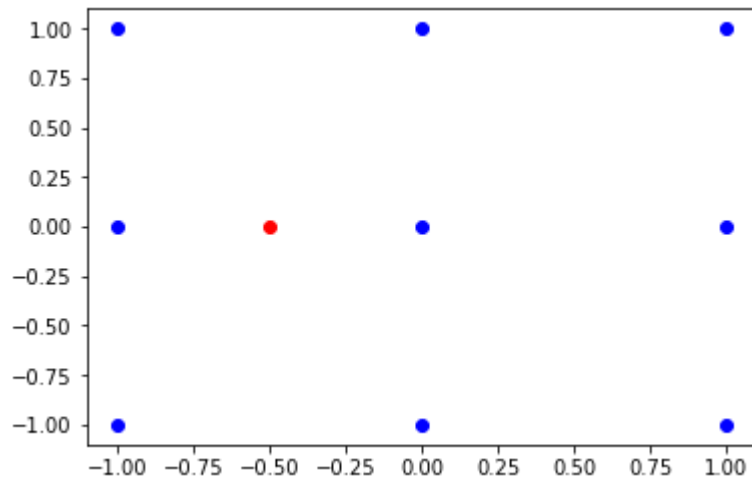
最近的3个点的坐标:

[[-1 0]

[ 0 0]

[-1 -1]]

[<matplotlib.lines.Line2D at 0x18079e39f98>]



## 4. 预言一个新的点的类别(class)

写一个函数实现:预言一个新点的类别.

找出距离p点最近的k个邻居的索引值;  
选出这些邻居中落在各类的次数("类似词语出现的频率")

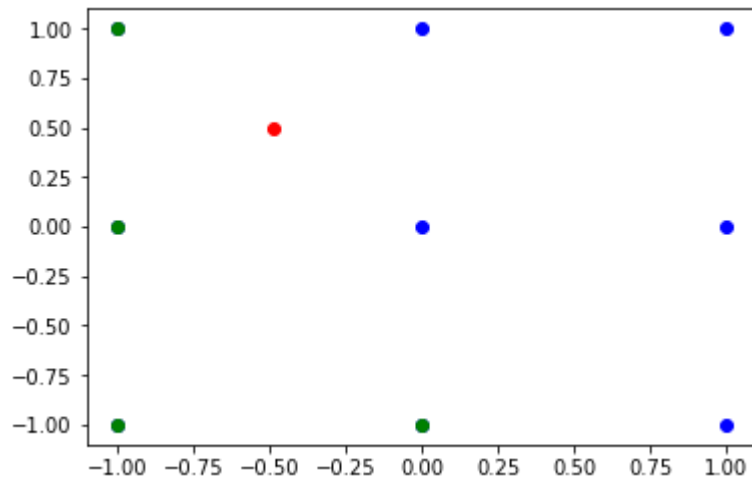
```
def knn_predict(p, points, outcomes, k=3):
    """返回新点p的类别."""
    ind = find_nn(p, points, k)
    #print("ind: ",ind)
    return majority_vote(outcomes[ind])

# outcomes为已知点points的类别
outcomes = np.array([0,0,0,0,1,1,1,1,1])
p = np.array([-0.49, .5])
points = np.array([[-1,-1], [-1,0], [-1,1], [0,-1], [0,0], [0,1], [1,-1], [1,0], [1,1]])
res = knn_predict(p, points,outcomes,3)
print("所属类别:",res)

#作图
plt.plot(points[:,0],points[:,1], "bo")
plt.plot(points[4,0],points[4,1], "go")
plt.plot(p[0],p[1], "ro")
```

所属类别: 1

[<matplotlib.lines.Line2D at 0x18079e81e80>]



## 5. 产生数据

---

end points:

bivariate:

ipstats 模块

```
# rvs(): 随机变量  
ss.norm(0,1).rvs((5,2))
```

```
array([[ 0.83069181, -0.62347007],  
       [-0.2725449 ,  0.11232394],  
       [-1.11716573, -0.44054168],  
       [ 0.45781264,  1.3071023 ],  
       [ 1.23865135,  0.83660122]])
```

```
ss.norm(1,1).rvs((5,2))
```

```
array([[ 1.35577686,  0.39040978],  
       [-0.66636033,  0.93560858],  
       [-0.41215857,  1.84704737],  
       [ 0.1551123 , -1.05379079],  
       [ 0.87793387, -0.03557217]])
```

```
np.concatenate((ss.norm(0,1).rvs((5,2)), ss.norm(1,1).rvs((5,2))), axis =0)
```

```
array([[ -0.4071305 ,  1.0495255 ],
       [ -3.45917693, -0.67421897],
       [ -0.2545249 , -1.73763083],
       [  0.76165822,  0.06027817],
       [  0.31492657,  0.41800532],
       [  3.23131752,  1.5114335 ],
       [  1.25727685,  0.0283415 ],
       [  0.75631692,  1.12605519],
       [  2.44503412,  1.44955582],
       [  1.55355979,  0.15840327]])
```

```
def generate_synth_data(n=50):
    points = np.concatenate((ss.norm(0,1).rvs((n,2)), ss.norm(1,1).rvs((n,2))), axis
=0)
    outcomes = np.concatenate((np.repeat(0,n),np.repeat(1,n)))
    return (points, outcomes)
```

```
generate_synth_data(n=50)
```

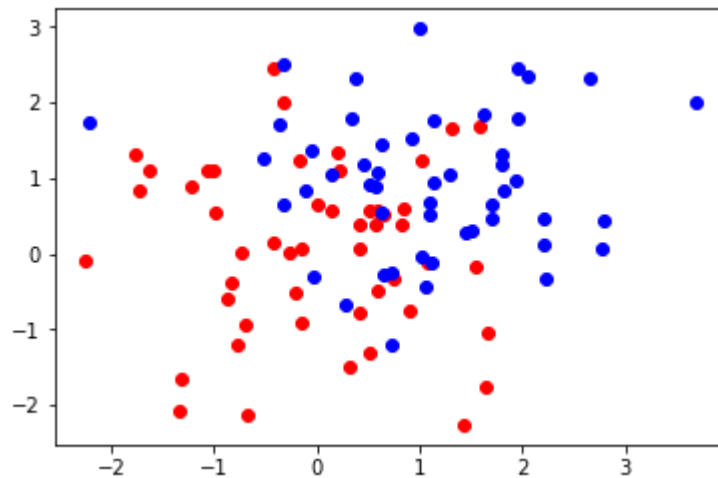
```
(array([[ -0.16783697,  0.02050534],
       [  0.33780707, -1.85746227],
       [  1.1502792 ,  0.41800664],
       [  0.44686681, -0.71024393],
       [  0.2298997 ,  0.07213386],
       [ -0.8118586 ,  2.40017804],
       [  1.58433468, -1.39424132],
       [ -0.24241004, -0.04255055],
       [  0.41714192, -0.51050465],
       [ -0.5280403 , -0.65786153],
       [ -1.57055482,  1.27481566],
       [  0.62697621,  0.26311523],
       [ -1.43334422,  0.7390689 ],
       [  1.67809832, -0.54769948],
       [ -1.16425757,  0.50000568],
       [  0.3132702 , -0.26666044],
       [  0.67253587, -0.1422316 ],
       [  0.50244811, -1.19014203],
       [ -0.4274232 , -0.26463046],
       [  1.79649483, -1.32868628],
       [  1.13115787,  0.40142446],
       [ -0.19614848, -0.22420655],
       [ -0.90000798, -1.35075547],
```

[ 0.94683432, 0.67866955],  
[ 1.86555968, -0.46159701],  
[ 0.43713084, -1.99728955],  
[ 1.19474333, -0.14155465],  
[-0.45634546, -0.32428328],  
[-1.48773399, 1.06669066],  
[ 0.3490665 , 0.2199291 ],  
[ 0.47055561, -0.39828232],  
[-0.06526523, 0.11699479],  
[-1.32039946, -0.15029049],  
[-0.47599881, -1.07159337],  
[ 0.96077185, 1.20452941],  
[ 0.60819762, 0.02412181],  
[-1.0173916 , -0.67349799],  
[-1.23975311, -1.04363138],  
[ 0.94641183, 0.74220721],  
[-0.95052702, 0.38768245],  
[-1.59797228, -0.38475813],  
[ 0.19346684, -0.65746161],  
[ 1.56409047, 0.28242497],  
[ 0.6899779 , -0.38342675],  
[ 0.46711867, -1.59927686],  
[-0.32635659, -0.54757973],  
[-0.81629077, -0.90463963],  
[ 1.19953136, -0.42577912],  
[ 0.88766725, 0.64721389],  
[-0.68097159, 0.95144207],  
[ 0.15045745, 1.77308766],  
[ 3.04339892, -0.34359456],  
[ 0.56568942, 0.50108106],  
[ 1.09376479, -0.03832559],  
[ 0.39485443, 1.0304349 ],  
[ 1.36046384, 1.75720897],  
[ 2.5963883 , 2.95865808],  
[ 1.71715505, 1.83740353],  
[ 1.023666 , 2.46374039],  
[ 1.14120557, 0.45604872],  
[ 0.82877602, 1.04832503],  
[ 1.31745272, -0.29050699],  
[ 1.46701593, 0.03811428],  
[-0.62785548, 2.0345153 ],  
[ 1.55931117, 2.76731343],  
[ 0.09051937, -0.1641055 ],  
[ 0.76399475, 1.64064433],  
[ 0.35090569, 2.62914281],  
[ 2.17176319, 1.65748757],  
[ 0.19211115, -0.47875665],  
[ 0.05048023, 0.64249643],  
[-0.09274217, 0.51781046],  
[ 1.66872886, 0.93564912],  
[ 0.75201328, 1.36039831],  
[ 0.7924292 , 0.05727138],  
[ 0.10401508, 1.94239822],

```
[ 1.20988334,  1.82051461],  
[ 0.88733247,  1.87191994],  
[ 2.04219745, -1.21850758],  
[ 1.9898411 , -0.20849328],  
[ 0.41398302,  0.70738275],  
[ 1.84098048,  1.54562855],  
[-0.31238646,  1.36357364],  
[-0.86696625,  0.11060323],  
[ 1.38585139, -0.33003332],  
[ 0.70032967, -0.75433882],  
[ 0.86737276,  0.97686573],  
[-0.05449175,  1.5307324 ],  
[ 0.88908613,  1.21785863],  
[-0.70619254, -0.87929872],  
[ 0.51253895,  1.16199514],  
[ 2.27498099,  3.11982834],  
[ 3.25427128,  1.29038675],  
[ 1.67351004, -0.38864826],  
[ 1.60965757,  0.49361361],  
[ 1.06842001,  0.97564107],  
[-0.17121087,  2.61243406],  
[-1.03616523,  1.62495132],  
[-0.57657601,  1.5198456 ],  
[-1.17619214,  1.64543992]]),  
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,  
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,  
       0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,  
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,  
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]))
```

```
points, outcomes = generate_synth_data(n=50)
```

```
plt.figure()
n = 50
plt.plot(points[:n,0], points[:n,1], "ro")
plt.plot(points[n:,0], points[n:,1], "bo")
plt.savefig("bivaradata.pdf")
```



## 6. 制作预测Grid

Learn how to make a prediction grid

Learn how to use enumerate

Learn how to use NumPy meshgrid

```
def make_pred_grid(predictors, outcomes, limits, h, k):
    (x_min, x_max, y_min, y_max) = limits
    xs = np.arange(x_min, x_max, h) # h, 步长
    ys = np.arange(y_min, y_max, h)
    xx, yy = np.meshgrid(xs, ys)

    pred_grid = np.zeros(xx.shape, dtype = int)
    for i, x in enumerate(xs):
        for j, y in enumerate(ys):
            p = np.array([x, y])
            pred_grid[j, i] = knn_predict(p, predictors, outcomes, k)

    return (xx, yy, pred_grid)
```

## 7. 对格点作图

Learn how to plot the prediction grid

Learn about the bias-variance tradeoff

```
# 可下载
def plot_pred_grid (xx, yy, prediction_grid, filename):
    """ Plot KNN predictions for every point on the grid."""
    from matplotlib.colors import ListedColormap
    background_colormap = ListedColormap (["hotpink", "yellowgreen", "lightskyblue" ])
    observation_colormap = ListedColormap (["red", "blue", "green"])
    plt.figure(figsize =(10,10))
    plt.pcolormesh(xx, yy, prediction_grid, cmap = background_colormap, alpha = 0.5)
```

```

plt.scatter(predictors[:,0], predictors[:,1], c = outcomes, cmap =
observation_colormap, s = 50)
plt.xlabel("x1"); plt.ylabel("x2")
plt.xticks(); plt.yticks()
plt.xlim(np.min(xx), np.max(xx))
plt.ylim(np.min(yy), np.max(yy))
plt.savefig(filename)

```

```

(predictors, outcomes) = generate_synth_data()

```

```

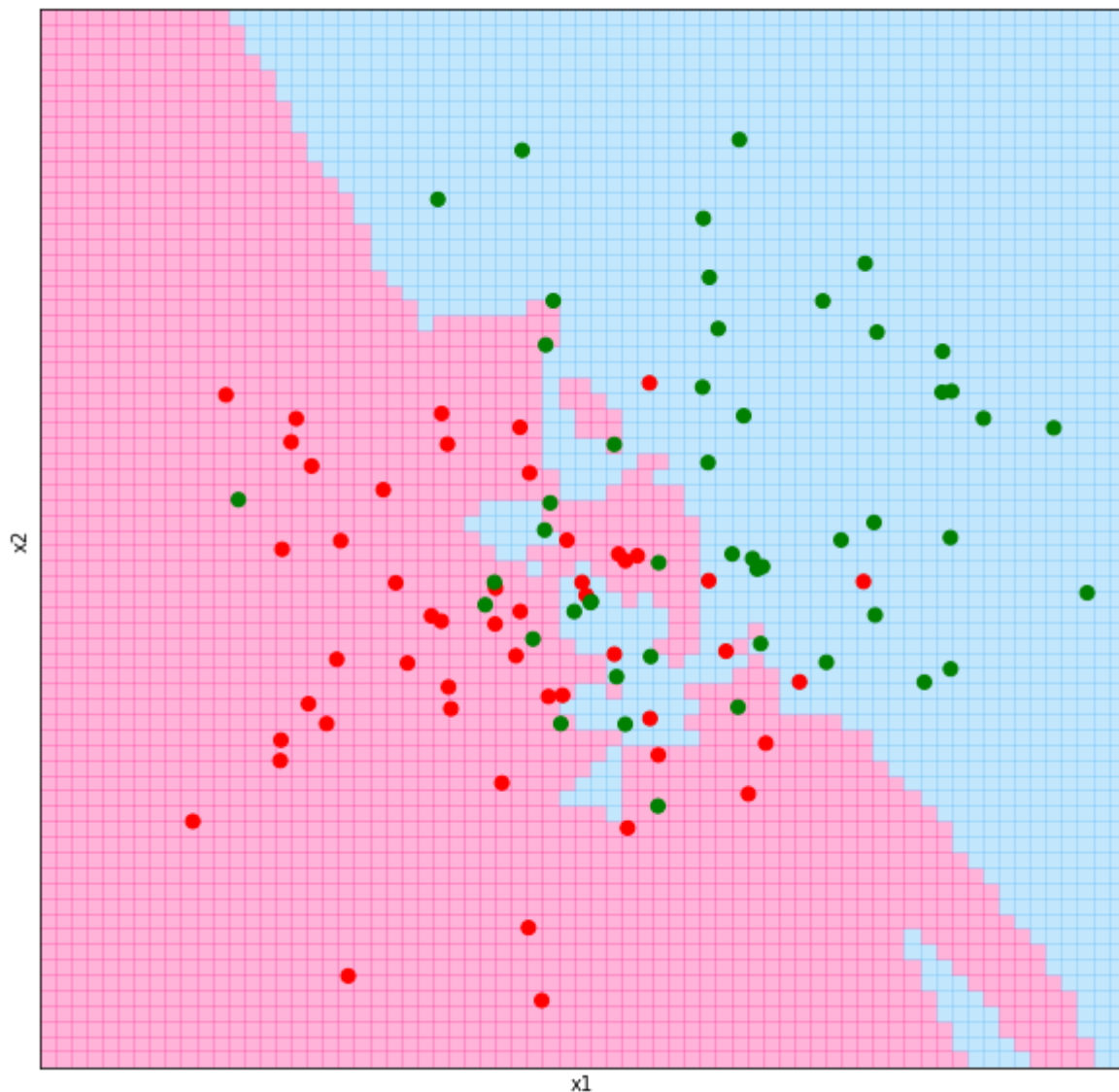
k = 5 ; filename = "knn_synth_5.pdf"
limits = (-3,4,-3,4) ; h = 0.1

```

```

(xx,yy, pred_grid) = make_pred_grid(predictors,outcomes,limits,h,k)
plot_pred_grid(xx,yy, pred_grid, filename)

```

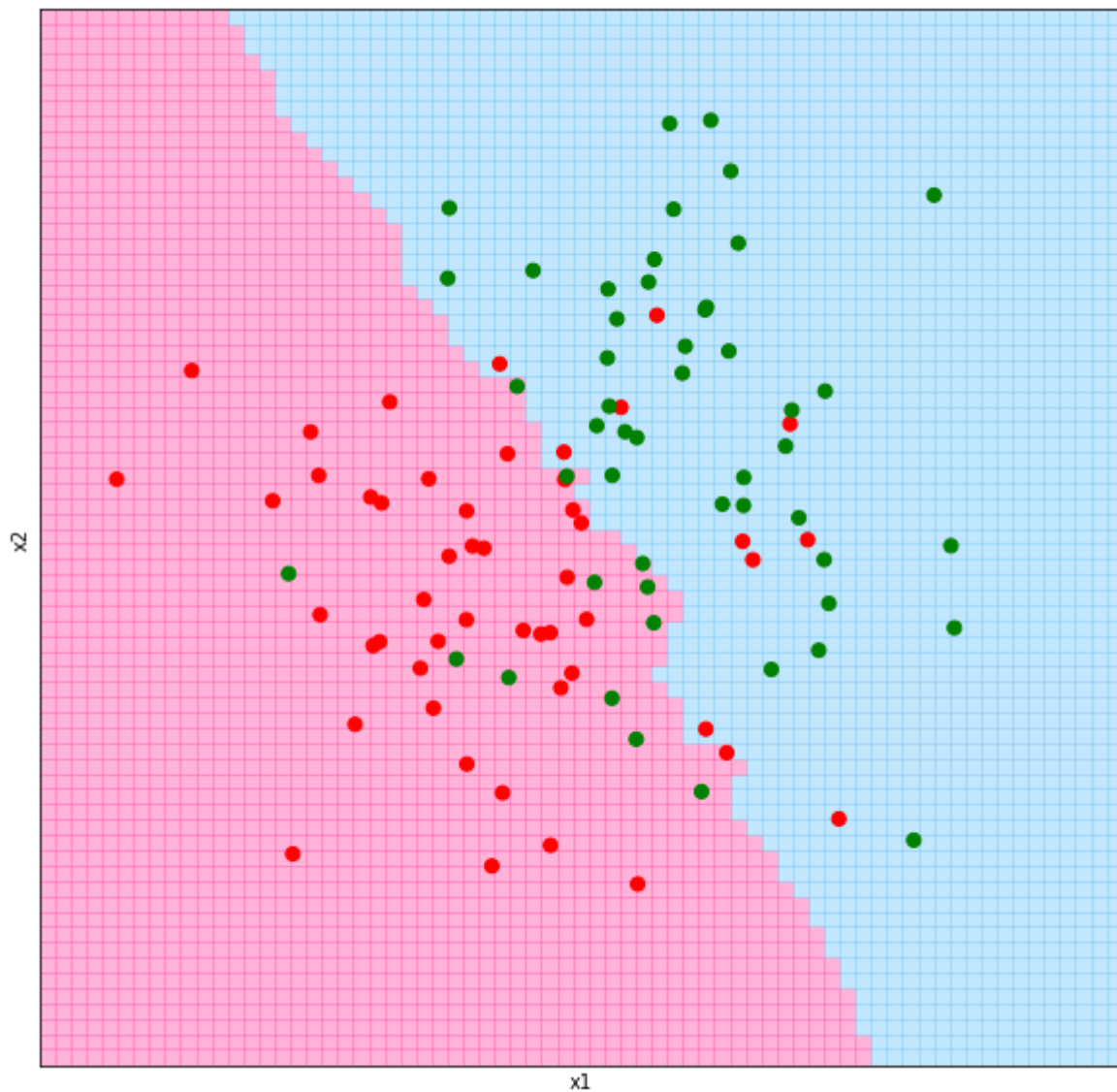




```
(predictors, outcomes) = generate_synth_data()

k = 13 ; filename = "knn_synth_13.pdf"
limits = (-3,4,-3,4) ; h = 0.1

(xx,yy, pred_grid) = make_pred_grid(predictors,outcomes,limits,h,k)
plot_pred_grid(xx,yy, pred_grid, filename)
```



## 8. Scikit-learn的使用

```
import pandas as pd
# 生成数据集：x中每个样本仅有一个特征.
X_train = pd.DataFrame([ [0], [1], [2], [3] ])
y_train = [0, 0, 1, 1]
X_train
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	0
0	0
1	1
2	2
3	3

```
y_train
```

```
[0, 0, 1, 1]
```

导入SciKit-Learn的 KNeighbors分类器.

```
from sklearn.neighbors import KNeighborsClassifier
model = KNeighborsClassifier(n_neighbors=3)
```

当我们拟合模型时,我们需要同时提供样本的特征和标签.

标签矢量应该为一个形状为(n\_samples,)的数组, 它应该包括每一个训练样本的标签.

下面是KNeighborsClassifier 类的几个参数(都是可选参数):

**n\_neighbors** : 邻居数目. 类别为2时,往往将n\_neighbors的值取为奇数. 尤其是我们用均匀权重时..  
**weights** : 每个邻居的"投票次数". 一般设每个邻居有相同的权重值  
**algorithm** : 我们可以选择搜索训练集的优化方法以找到最近邻居.

```
model.fit(X_train, y_train)
```

```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=3, p=2,
                    weights='uniform')
```

```
# 传入一个df或者一个数组
model.predict([[1.1]])
```

```
array([0])
```

```
model.predict([[1.1], [3.3]])
```

```
array([0, 1])
```

```
model.predict_proba([[0.9], [0.3]])
```

```
array([[0.66666667, 0.33333333],
       [0.66666667, 0.33333333]])
```

```
model.score([[0.9], [0.3]], [0, 1])
```

```
0.5
```

## 9. 应用kNN模型

应用我们自己写的kNN分类器到一个真实的数据集。  
对比我们的kNN分类器和scikit-learn模块的kNN分类器的表现。

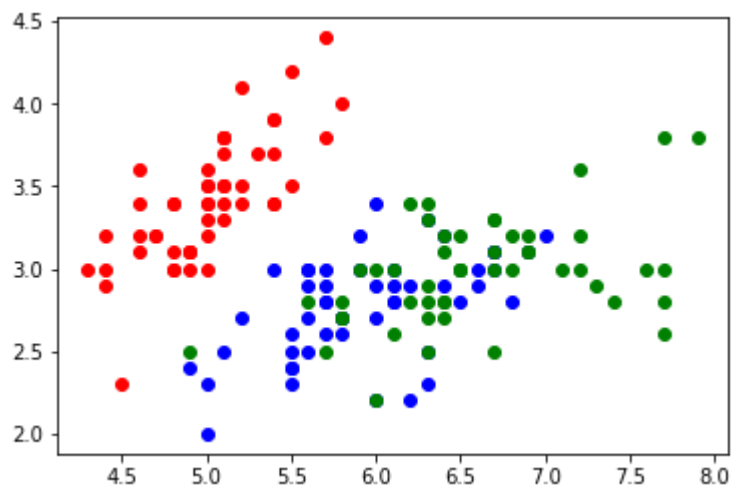
数据集: 150朵鸢尾花(Iris):共有三种,每种的数量为50.

对每一朵花,有如下变量(covariates):

花萼(sepal)长度, 花萼宽度;  
花瓣(petal)长度, 花瓣宽度.

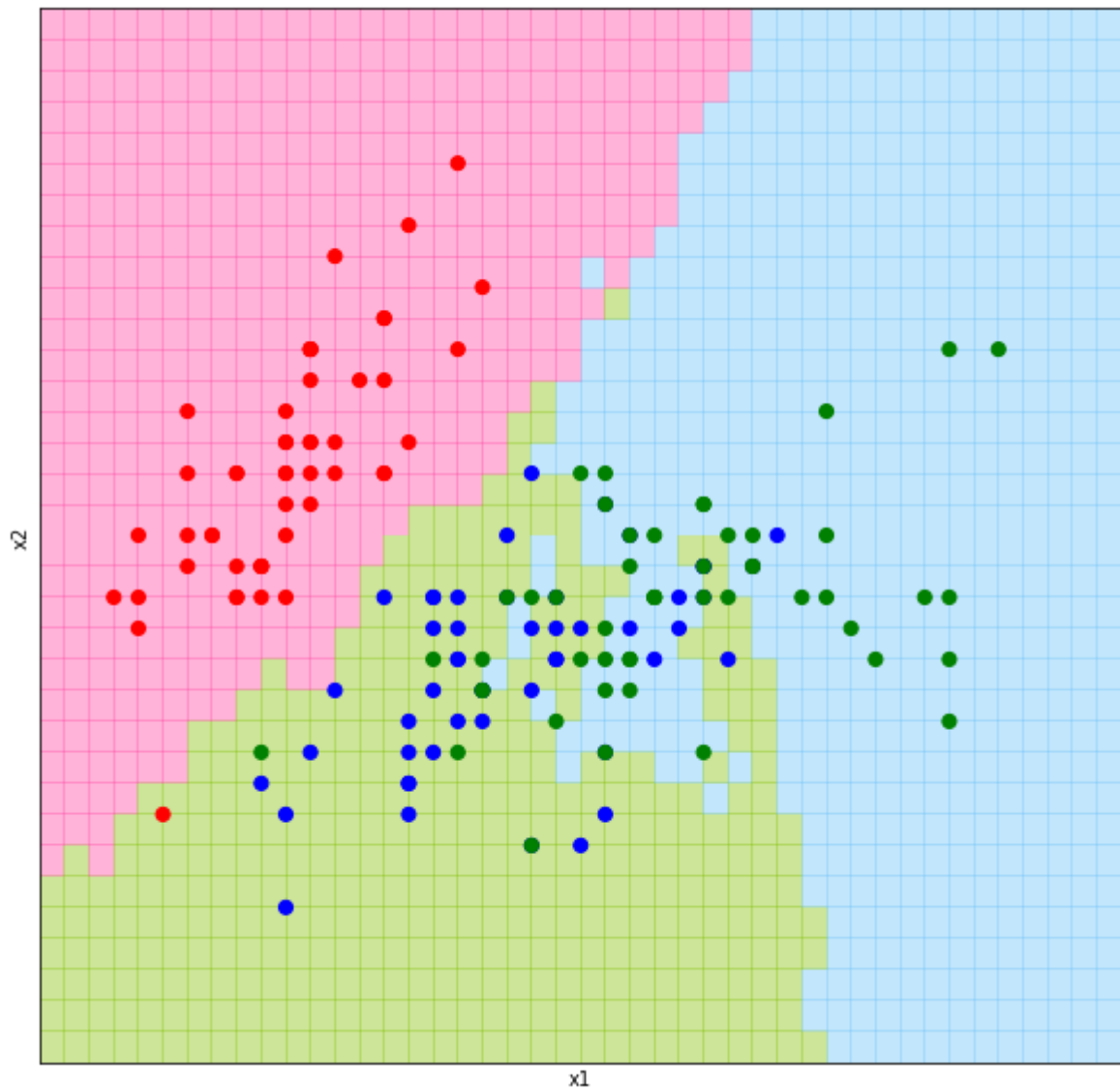
```
from sklearn import datasets
iris = datasets.load_iris()

#iris
predictors = iris.data[:,0:2]
outcomes = iris.target
#print(outcomes == 0)
#print(predictors[outcomes==0][:,0])
plt.plot(predictors[outcomes==0][:,0], predictors[outcomes==0][:,1] , "ro")
plt.plot(predictors[outcomes==1][:,0], predictors[outcomes==1][:,1] , "bo")
plt.plot(predictors[outcomes==2][:,0], predictors[outcomes==2][:,1] , "go")
plt.savefig("iris.svg")
```



```
k = 5 ; filename = "iris_grid.pdf";
limits = (4, 8.5, 1.5, 5) ; h = 0.1

(xx,yy, pred_grid) = make_pred_grid(predictors,outcomes,limits,h,k)
plot_pred_grid(xx,yy, pred_grid, filename)
```



```
from sklearn.neighbors import KNeighborsClassifier
```

```
# 建立knn模型
```

```
knn = KNeighborsClassifier(n_neighbors = 5)
```

```
knn.fit(predictors,outcomes)
```

```
sk_predictions = knn.predict(predictors)
```

```
sk_predictions.shape
```

```
(150,)
```

```
sk_predictions[:10]
```

```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0])
```

```
my_predictions = np.array([knn_predict(p,predictors, outcomes, 5) for p in predictors])
my_predictions
```

```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0,
       0, 0, 0, 0, 0, 2, 2, 2, 1, 2, 1, 2, 1, 1, 1, 1, 2, 1, 1, 1, 1,
       1, 2, 1, 1, 1, 1, 2, 1, 2, 2, 1, 2, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2,
       2, 2, 2, 1, 1, 2, 2, 2, 2, 1, 2, 1, 2, 2, 2, 2, 1, 1, 2, 2, 2,
       2, 2, 1, 2, 2, 2, 2, 2, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

```
my_predictions == sk_predictions
```

```
array([ True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True, False,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True, False,  True,  True,  True,
        True,  True,  True,  True, False,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True, False,  True,  True,  True, False])
```

```
# 两种算法的对比
print(100 * np.mean(my_predictions == sk_predictions))
```

```
96.0
```

```
# 计算准确率
print(100 * np.mean(my_predictions == outcomes))
print(100 * np.mean(sk_predictions == outcomes))
```

```
84.66666666666667
83.33333333333334
```

## 小结:

1. kNN is particularly useful when no other model fits your data well, 因为它是一个不需要参数的分类方法。例如,你不需要考虑你的数据是线性可分还是线性不可分。
2. 要想用kNN算法,我们的数据必须是可测的(数据集上有距离可以定义出来)。

## 10. kNN应用(2)

mglearn.plots.plot\_classification()

```
import mglearn
import matplotlib.pyplot as plt
from sklearn.datasets import load_boston

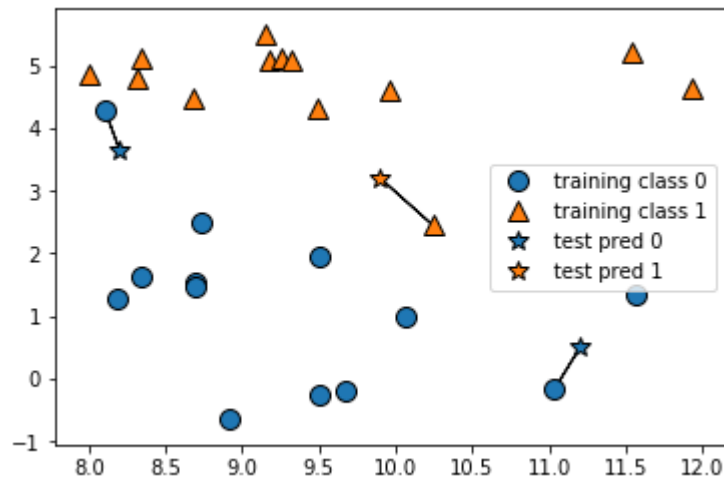
boston = load_boston()

print("数据形状:{}".format(boston.data.shape))

# 生成扩展数据集
X, y = mglearn.datasets.load_extended_boston()
print("X.shape:{}".format(X.shape))

mglearn.plots.plot_knn_classification(n_neighbors=1)
plt.show()
```

```
数据形状:(506, 13)
X.shape:(506, 104)
```



(2)计算决策边界.

```
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier
X,y = mglearn.datasets.make_forge()
X_train, X_test, y_train, y_test = train_test_split(X,y, random_state=0)

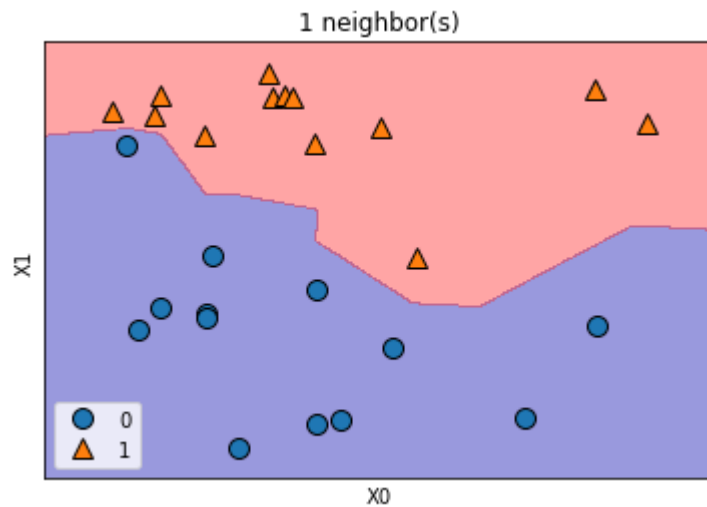
n_neighbors =1
# KNeighborsClassifier类的实例化
clf = KNeighborsClassifier(n_neighbors= n_neighbors)
clf.fit(X_train, y_train)
print("测试集预测: {}".format(clf.predict(X_test)))
print("测试集准确度: {:.3f}".format(clf.score(X_test,y_test)))

clf = KNeighborsClassifier(n_neighbors=n_neighbors).fit(X,y)
#边界
mglearn.plots.plot_2d_separator(clf, X, fill=True, eps=0.5, alpha=0.4)
# 散点图
mglearn.discrete_scatter(X[:,0],X[:,1],y)
plt.title("{} neighbor(s)".format(n_neighbors))
plt.xlabel("x0")
plt.ylabel("x1")
plt.legend(loc=3)
plt.show()
```

测试集预测: [1 0 1 0 1 0 0]

测试集准确度: 0.857





k越大,边界越光滑.

k越小,模型越复杂.(复杂度大)

k越大,模型越简单.

k极大,所有测试数据对应预测值都一样.

(3) 测试性能和准确度.

```
from sklearn.datasets import load_breast_cancer

cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, stratify=cancer.target, random_state=6)

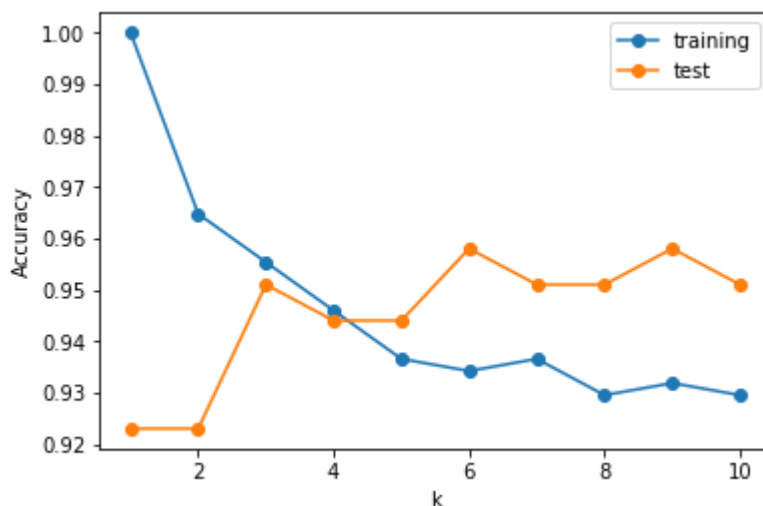
training_accuracy = []
test_accuracy = []

# try n_neighbors from 1 to 10
neighbors = range(1,11)

for n_neighbors in neighbors:
    # build the model
    clf = KNeighborsClassifier(n_neighbors=n_neighbors)
    clf.fit(X_train,y_train)
    #record training set accuracy
    training_accuracy.append(clf.score(X_train,y_train))
    #record generalization accuracy
    test_accuracy.append(clf.score(X_test,y_test))

plt.plot(neighbors,training_accuracy, "o-",label="training")
plt.plot(neighbors,test_accuracy, "o-",label="test")
plt.ylabel("Accuracy")
plt.xlabel("k")
plt.legend()
```

<matplotlib.legend.Legend at 0x18000038c50>



k越小,模型越复杂.(复杂度大,过拟合: 对于训练集的预测是完美的.但对于测试集的预测表现很差劲. Too complex Model!)

随着k增大,模型越来越简单. 训练集上的准确度降低.但测试集上的准确度逐渐增大.

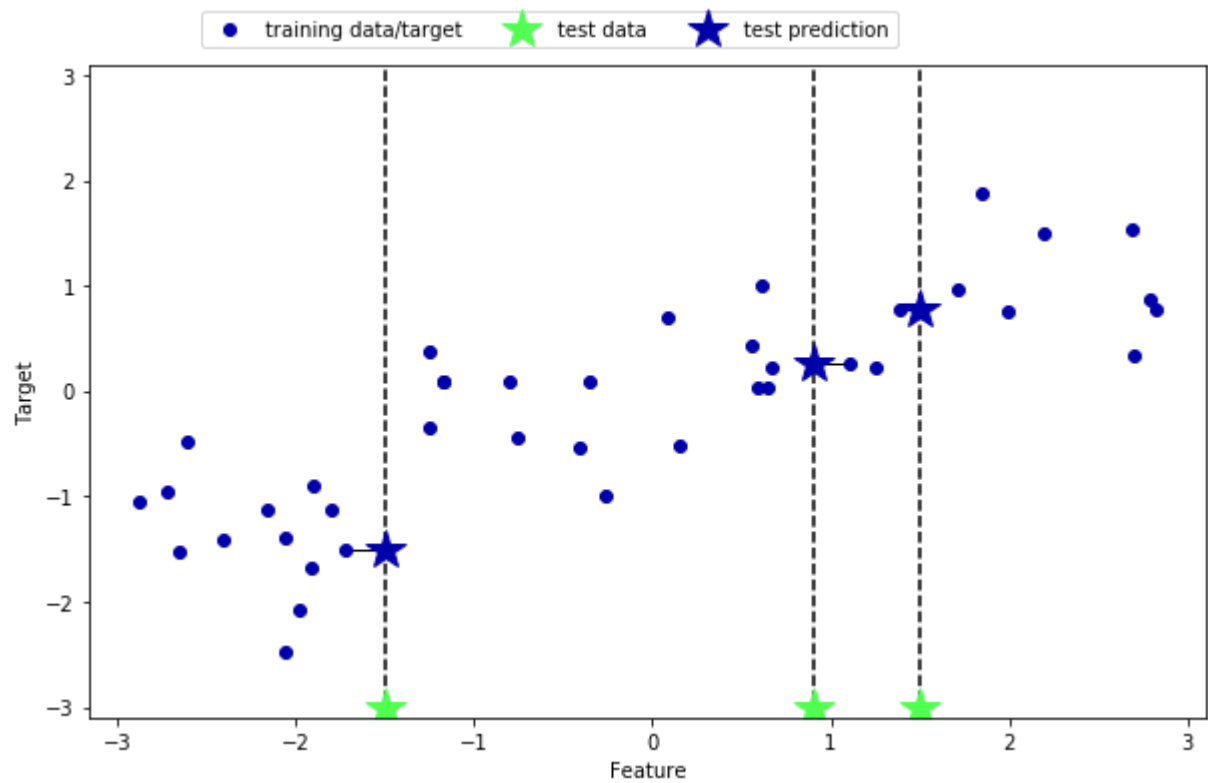
当k过大时,测试集上的准确度甚至比单邻居情形更惨. 表现很好的模型是k位于[1,10]之间的某个值的哪些模型. (注意:这里的模型表现都还不错!)

当k取得极其大,所有测试数据对应预测值都一样.

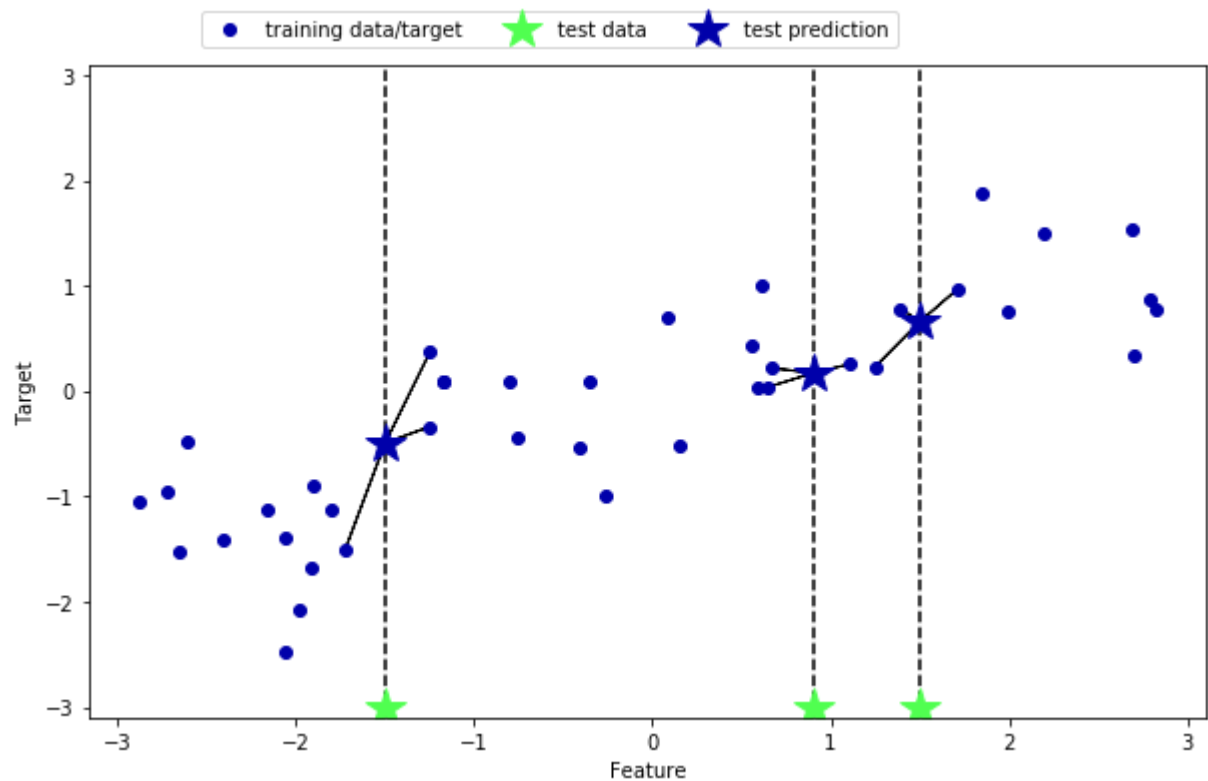
## 11. kNN回归算法

```
from sklearn.model_selection import train_test_split
from sklearn.datasets import load_breast_cancer
#import matplotlib.pyplot as plt
#import mglearn

X,y = mglearn.datasets.make_forge()
# 数据集分割
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
# 选单个邻居数为1时, 目标值就是其最近邻居之目标值. (这就是k=1时的kNN回归)
mglearn.plots.plot_knn_regression(n_neighbors=1)
plt.show()
```



```
X,y = mglearn.datasets.make_forge()
# 数据集分割
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
# 选单个邻居数为3时，目标值就是其最近3个邻居之目标值之平均值。(这就是k=3时的kNN回归)
mglearn.plots.plot_knn_regression(n_neighbors=3)
plt.show()
```



```
from sklearn.neighbors import KNeighborsRegressor
X,y = mglearn.datasets.make_wave(n_samples=40)
# 分割数据集
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
# 实例化模型,k=3
reg = KNeighborsRegressor(n_neighbors=3)
# 利用数据拟合模型
reg.fit(X_train,y_train)
```

```
KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=3, p=2,
                    weights='uniform')
```

```
# 现在在新的数据集上做预测
print("X_test:",X_test)
print("Test set predictions:\n{}".format(reg.predict(X_test)))
```

```
x_test: [[-1.24713211]
 [ 0.67111737]
 [ 1.71105577]
 [-2.06388816]
 [-2.87649303]
 [-1.89957294]
 [ 0.55448741]
 [ 2.81945911]
 [-0.40832989]
 [-2.72129752]]
Test set predictions:
[-0.05396539  0.35686046  1.13671923 -1.89415682 -1.13881398 -1.63113382
 0.35686046  0.91241374 -0.44680446 -1.13881398]
```

## 拟合优度

利用score()方法评估模型. 对回归算法,它返回判定系数 $R^2$ 之值. (coefficient of determination),又称拟合优度.

$R^2$ 是测量回归模型好坏的一个量. 取值在[0,1]之间.  $R^2 = 1$ 表示模型可以做完美的预测;  $R^2 = 0$ 表示该模型只能做出预测值mean(y\_train).

设一数据集包括 $y_1, \dots, y_n$ 共n个观察值, 相对应的模型预测值分别为 $f_1, \dots, f_n$ .

定义残差 $e_i = y_i - f_i$ , 平均观察值为

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i.$$

决定系数定义为

$$R^2 \equiv 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}.$$

其中,总平方和

$$SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2$$

回归平方和

$$SS_{\text{reg}} = \sum_i (f_i - \bar{y})^2,$$

残差平方和

$$SS_{\text{res}} = \sum_i (y_i - f_i)^2 = \sum_i e_i^2,$$

```
print("测试集拟合优度:{:.3f}".format(reg.score(X_test,y_test)))
```

```
测试集拟合优度:0.834
```

## kNN回归分析

```
#如果数据仅有一个特征,利用array.reshape(-1, 1)改变数组形状;
#如果数据中仅包含一个样本,则可利用array.reshape(1, -1)改变数组形状.
line = np.linspace(-3,3, 1000).reshape(-1,1)
```

```

n_neighbors = 1 # 可改变k值
reg = KNeighborsRegressor(n_neighbors=n_neighbors)
reg.fit(X_train,y_train)
plt.plot(line[:,0], reg.predict(line))
plt.plot(X_train[:,0],y_train, "o", c="r")
plt.plot(X_test[:,0],y_test, "v", c="b")

plt.title("{} neighbor(s)\n train score:{:.2f} test score: {:.2f}".format(n_neighbors,
reg.score(X_train,y_train),

    reg.score(X_test,y_test)))
plt.xlabel("Feature")
plt.ylabel("Target")
plt.legend(["Predictions", "Training data/target", "Test data/target"])

```

<matplotlib.legend.Legend at 0x1807b32c358>

