大家好,这篇是有关台大机器学习课程作业五的详解。

我的github地址:

https://github.com/Doraemonzzz

个人主页:

http://doraemonzzz.com/

作业地址:

https://www.csie.ntu.edu.tw/~htlin/course/ml15fall/

参考资料:

https://blog.csdn.net/a1015553840/article/details/51085129

http://www.vynguyen.net/category/study/machine-learning/page/6/

http://book.caltech.edu/bookforum/index.php

http://beader.me/mlnotebook/

https://blog.csdn.net/qian1122221/article/details/50130093

Problem 1

回顾下问题的形式

$$egin{aligned} \min_{w,b,\xi} : rac{1}{2} w^T w + C \sum_{n=1}^N \xi_n \ ext{subject to: } y_n(w^T x_n + b) \geq 1 - \xi_n \ \xi_n \geq 0 (n = 1, \dots, N) \end{aligned}$$

 x_n,y_n 为变量,C为人为设定的超参数,其余量均为参数,注意 $w\in\mathbb{R}^d$,所以我们的参数有

$$w=(w_1,\ldots,w_d),\xi_1,\ldots,\xi_N,d$$

一共d+N+1个。限制条件为

$$y_n(w^Tx_n + b) \ge 1 - \xi_n$$

 $\xi_n > 0 (n = 1, \dots, N)$

一共有2N个。

Problem 2

首先作图看下

```
# -*- coding: utf-8 -*-
"""

Created on Sat Mar 23 13:11:34 2019

@author: qinzhen
```

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn import svm

####Problem 2

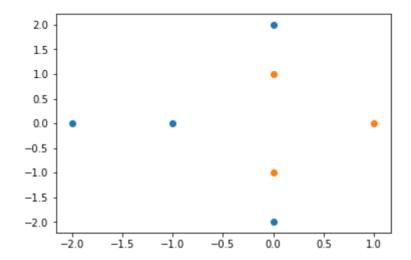
#原始图

x = np.array([[1, 0],[0, 1],[0, -1],[-1, 0],[0, 2],[0, -2],[-2, 0]])

z = np.array([-1, -1, -1, +1, +1, +1])

x1 = x[z>0][:, 0]
y1 = x[z>0][:, 1]
x2 = x[z<0][:, 0]
y2 = x[z<0][:, 1]

plt.scatter(x1,y1)
plt.scatter(x2,y2)
plt.show()
```



可以看到,如果用二次曲线的话,应该可以分类,现在做特征转换之后的图像。

转换之后的标记为+1的点为

$$z_4 = (5, -2), z_5 = (7, -7), z_6 = (7, 1), z_7 = (7, 1)$$

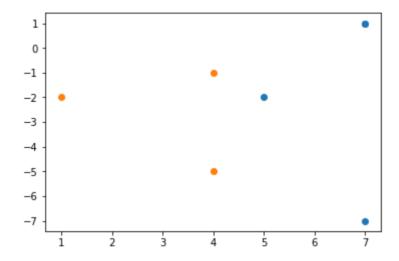
转换之后的标记为+1的点为

$$z_1=(1,-2), z_2=(4,-5), z_3=(4,-1)$$

```
#特征转换之后的图
def phi_1(x):
    return x[1] ** 2 - 2 * x[0] + 3

def phi_2(x):
    return x[0] ** 2 - 2 * x[1] - 3

X = []
```



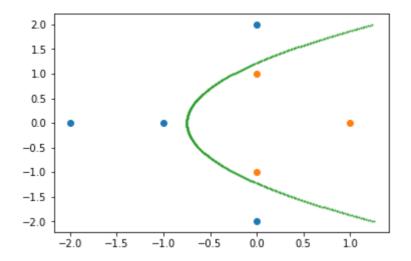
从这个图像中可以看出,最大间隔分类器为 $\phi_1(x)=4.5$,将 $\phi_1(x)=x_2^2-2x_1+3$ 带入可得最大间隔分类器为

$$x_2^2 - 2x_1 + 3 = 4.5$$
$$x_1 = \frac{x_2^2 - 1.5}{2}$$

最后看下曲线的图。

```
#曲线图
y3 = np.arange(-2, 2, 0.01)
x3 = np.array([(i * i - 1.5) / 2 for i in y3])

plt.scatter(x1, y1)
plt.scatter(x2, y2)
plt.scatter(x3, y3, s=1)
plt.show()
```



利用sklearn处理即可,这里设置参数shrinking=False,参数含义如下:

https://stats.stackexchange.com/questions/24414/svm-options-in-scikit-learn

```
clf = svm.SVC(kernel='poly', degree=2, coef0=1, gamma=1, C=1e10, shrinking=False)
clf.fit(x, z)
```

```
SVC(C=10000000000.0, cache_size=200, class_weight=None, coef0=1,
  decision_function_shape='ovr', degree=2, gamma=1, kernel='poly',
  max_iter=-1, probability=False, random_state=None, shrinking=False,
  tol=0.001, verbose=False)
```

看下哪几个向量为支持向量。

```
clf.support_
```

```
array([1, 2, 3, 4, 5])
```

这说明第2到6个向量均为支持向量,再来看下对偶问题的系数。

```
clf.dual_coef_
```

```
array([[-0.64491963, -0.76220325, 0.88870349, 0.22988879, 0.2885306]])
```

这些系数分别支持向量对应的系数,非支持向量对应的系数为0,这里还要注意一点,对偶问题的系数为 $y_n\alpha_n$,所以如果我们要得到原系数,就要乘以 y_n

```
z[clf.support_] * clf.dual_coef_[0]
```

```
array([0.64491963, 0.76220325, 0.88870349, 0.22988879, 0.2885306])
```

所以

 $(\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5,\alpha_6,\alpha_7) = (0,0.64491963,0.76220325,0.88870349,0.22988879,0.2885306,0)$ 支持向量为

$$x_2, x_3, x_4, x_5, x_6$$

Problem 4

为了求得曲线方程,我们需要利用以下几个式子

$$egin{aligned} w &= \sum_{lpha_n^*>0} y_n lpha_n^* z_n^T \ b &= y_s - w^T z_s \ g(x) &= ext{sign} \Big(\sum_{lpha_n^*>0} y_n lpha_n^* K(x_n,x) + b \Big) \end{aligned}$$

注意

$$K(x_n,x) = (1+x_n^Tx)^2$$

首先计算b, 可以直接获得:

```
b = clf.intercept_[0]
b
```

-1.6663314053609206

接着计算 $K(x_n, x) = (1 + x_n^T x)^2$, 首先找出支持向量:

```
x[clf.support_]
```

然后计算上式,记

$$x=(x^{(1)},x^{(2)})$$

那么每一项分别为:

$$egin{aligned} (1+x^{(2)})^2 \ (1-x^{(2)})^2 \ (1-x^{(1)})^2 \ (1+2x^{(2)})^2 \ (1-2x^{(2)})^2 \end{aligned}$$

最后计算 $\alpha_n y_n$, 直接调用即可:

```
clf.dual_coef_[0]
```

```
array([-0.64491963, -0.76220325, 0.88870349, 0.22988879, 0.2885306])
```

所以曲线方程为:

```
-0.64491963(1+x^{(2)})^2 - 0.76220325(1-x^{(2)})^2 + 0.88870349(1-x^{(1)})^2 + 0.22988879(1+2x^{(2)})^2 + 0.2885306(1-2x^{(2)})^2 - 1.6663314053609206 = 0
```

Problem 5

这里作图来看:

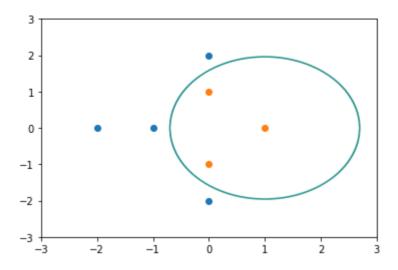
```
#点的数量
n = 1000
r = 3

#作点
a = np.linspace(-r, r, n)
b = np.linspace(-r, r, n)

#构造网格
A, B = np.meshgrid(a, b)
X = np.c_[A.reshape(-1, 1), B.reshape(-1, 1)]
label = np.reshape(clf.predict(X), A.shape)

#绘制等高线
plt.contour(A, B, label, 0)

plt.scatter(x1, y1)
plt.scatter(x2, y2)
plt.show()
```



可以看到, 图像和之前的抛物线是不一样的。

Problem 6

结合课件的推导, 我们可知

$$egin{aligned} L(R,c,\lambda) &= R^2 + \sum_{n=1}^N \lambda_n(||x_n-c||^2 - R^2) \ \lambda_n &\geq 0 \end{aligned}$$

所以在 $||x_n - c||^2 \le R^2$ 条件下

$$\sum_{n=1}^N \lambda_n(||x_n-c||^2-R^2) \leq 0 \ \max\{\sum_{n=1}^N \lambda_n(||x_n-c||^2-R^2)\} = 0$$

从而

$$\min_{R \in \mathbb{R}, c \in \mathbb{R}^d} \max_{\lambda_n \geq 0} L(R, c, \lambda) = \min_{R \in \mathbb{R}, c \in \mathbb{R}^d} \!\! R^2$$

Problem 7

将上述问题转化为对偶问题

$$\min_{R \in \mathbb{R}, c \in \mathbb{R}^d} \max_{\lambda_n \geq 0} L(R, c, \lambda) = \max_{\lambda_n \geq 0} \min_{R \in \mathbb{R}, c \in \mathbb{R}^d} L(R, c, \lambda)$$

所以现在可以对 $L(R,c,\lambda)$ 求无条件极值,分别求偏导可得

$$egin{aligned} rac{\partial L(R,c,\lambda)}{\partial c} &= rac{\partial [R^2 + \sum_{n=1}^N \lambda_n (||x_n-c||^2 - R^2)]}{\partial c} \ &= rac{\partial [R^2 + \sum_{n=1}^N \lambda_n (x_n^T x_n - 2x_n^T c + c^T c - R^2)]}{\partial c} \ &= rac{\partial [R^2 + \sum_{n=1}^N \lambda_n (x_n^T x_n - 2x_n^T c + c^T c - R^2)]}{\partial c} \ &= \sum_{n=1}^N \lambda_n rac{\partial (x_n^T x_n - 2x_n^T c + c^T c - R^2)}{\partial c} \ &= \sum_{n=1}^N \lambda_n (2c - 2x_n) \ &= 2(c \sum_{n=1}^N \lambda_n - \sum_{n=1}^N \lambda_n x_n) \end{aligned}$$

令 $\frac{\partial L(R,c,\lambda)}{\partial c}=0$ 可得

$$c\sum_{n=1}^N \lambda_n - \sum_{n=1}^N \lambda_n x_n = 0$$

如果

$$\sum_{n=1}^N \lambda_n
eq 0$$

那么

$$c = rac{\sum_{n=1}^{N} \lambda_n x_n}{\sum_{n=1}^{N} \lambda_n}$$

接着关于R求偏导

$$egin{aligned} rac{\partial L(R,c,\lambda)}{\partial R} &= rac{\partial [R^2 + \sum_{n=1}^N \lambda_n (||x_n - c||^2 - R^2)]}{\partial R} \ &= 2R - 2\sum_{n=1}^N \lambda_n R \end{aligned}$$

令 $\frac{\partial L(R,c,\lambda)}{\partial R}=0$ 可得

$$\sum_{n=1}^N \lambda_n = 1$$

结合这个条件,关于c的条件可以简化

$$c = rac{\sum_{n=1}^{N} \lambda_n x_n}{\sum_{n=1}^{N} \lambda_n} = \sum_{n=1}^{N} \lambda_n x_n$$

将 $\sum_{n=1}^N\lambda_n=1,c=\sum_{n=1}^N\lambda_nx_n$ 这两个条件带入 $L(R,c,\lambda)$,先带入 $\sum_{n=1}^N\lambda_n=1$

$$egin{aligned} L(R,c,\lambda) &= R^2 + \sum_{n=1}^N \lambda_n (||x_n - c||^2 - R^2) \ &= \sum_{n=1}^N \lambda_n ||x_n - c||^2 + R^2 - R^2 \sum_{n=1}^N \lambda_n \ &= \sum_{n=1}^N \lambda_n ||x_n - c||^2 \end{aligned}$$

再对 $\sum_{n=1}^{N}\lambda_{n}||x_{n}-c||^{2}$ 进行处理可得

$$egin{aligned} L(R,c,\lambda) &= \sum_{n=1}^{N} \lambda_{n} ||x_{n} - c||^{2} \ &= \sum_{n=1}^{N} \lambda_{n} (x_{n}^{T}x_{n} - 2x_{n}^{T}c + c^{T}c) \ &= \sum_{n=1}^{N} \lambda_{n} x_{n}^{T}x_{n} - 2(\sum_{n=1}^{N} \lambda_{n} x_{n}^{T})c + c^{T}c \sum_{n=1}^{N} \lambda_{n} \ &= \sum_{n=1}^{N} \lambda_{n} x_{n}^{T}x_{n} - 2(\sum_{n=1}^{N} \lambda_{n} x_{n}^{T})c + c^{T}c \end{aligned}$$

再带入 $c = \sum_{n=1}^N \lambda_n x_n$

$$egin{aligned} L(R,c,\lambda) &= \sum_{n=1}^N \lambda_n x_n^T x_n - 2c \sum_{n=1}^N \lambda_n x_n^T + c^T c \ &= \sum_{n=1}^N \lambda_n x_n^T x_n - 2(\sum_{n=1}^N \lambda_n x_n^T)(\sum_{n=1}^N \lambda_n x_n) + (\sum_{n=1}^N \lambda_n x_n^T)(\sum_{n=1}^N \lambda_n x_n) \ &= \sum_{n=1}^N \lambda_n x_n^T x_n - (\sum_{n=1}^N \lambda_n x_n^T)(\sum_{n=1}^N \lambda_n x_n) \end{aligned}$$

所以问题转换为

在条件
$$\sum_{n=1}^N \lambda_n=1, \lambda_n\geq 0$$
下,最小化 $f(\lambda)=\sum_{n=1}^N \lambda_n x_n^T x_n-(\sum_{n=1}^N \lambda_n x_n^T)(\sum_{n=1}^N \lambda_n x_n)$

这题是要利用 $z_n = \phi(x_n)$ 以及 $K(x_n, x_m)$ 来简化问题,先对 $f(\lambda)$ 进行处理

$$egin{aligned} f(\lambda) &= \sum_{n=1}^N \lambda_n x_n^T x_n - (\sum_{n=1}^N \lambda_n x_n^T) (\sum_{n=1}^N \lambda_n x_n) \ &= \sum_{n=1}^N \lambda_n x_n^T x_n - \sum_{n=1}^N \sum_{m=1}^N \lambda_n \lambda_m x_n^T x_m \end{aligned}$$

将 x_n 替换为 $z_n = \phi(x_n)$,然后代入 $K(x_n, x_m) = z_n^T z_m$ 可得

$$egin{aligned} f(\lambda) &= \sum_{n=1}^N \lambda_n z_n^T z_n - \sum_{n=1}^N \sum_{m=1}^N \lambda_n \lambda_m z_n^T z_m \ &= \sum_{n=1}^N \lambda_n K(x_n, x_n) - \sum_{n=1}^N \sum_{m=1}^N \lambda_n \lambda_m K(x_n, x_m) \end{aligned}$$

Problem 10

由Problem 6的推导过程我们可知,

$$\lambda_n(||x_n-c||^2-R^2)=0$$

 $n=1,\ldots,N$

这里讨论的是特征转换之后的问题, 所以上述问题可以修改为

$$\lambda_n(||z_n - c||^2 - R^2) = 0$$
$$n = 1, \dots, N$$

所以如果存在 $\lambda_i \neq 0$, 那么

$$||z_i - c||^2 - R^2 = 0$$

结合 $c=\sum_{n=1}^{N}\lambda_{n}z_{n}$,可得

$$egin{aligned} R^2 &= \left| \left| z_i - c
ight|
ight|^2 \ &= (z_i - \sum_{n=1}^N \lambda_n z_n)^T (z_i - \sum_{n=1}^N \lambda_n z_n) \ &= z_i^T z_i - 2 \sum_{n=1}^N \lambda_n z_n^T z_i + \sum_{n=1}^N \sum_{m=1}^N \lambda_n \lambda_m z_n^T z_m \ &= K(x_i, x_i) - 2 \sum_{n=1}^N \lambda_n K(x_n, x_i) + \sum_{n=1}^N \sum_{m=1}^N \lambda_n \lambda_m K(x_n, x_m) \end{aligned}$$

首先看下现在的问题,假设假设 $x_n \in \mathbb{R}^k$

$$egin{aligned} \min_{w,b,\xi} & rac{1}{2} w^T w + C \sum_{n=1}^N \xi_n^2 \ ext{subject to } y_n(w^T x_n + b) \geq 1 - \xi_n \end{aligned}$$

转换成hard-margin的关键问题在于把 $\frac{1}{2}w^Tw+C\sum_{n=1}^N\xi_n^2$ 写成 $\frac{1}{2}\tilde{w}^T\tilde{w}$

$$rac{1}{2}w^Tw + C\sum_{n=1}^N \xi_n^2 = rac{1}{2}(w^Tw + 2C\sum_{n=1}^N \xi_n^2)$$

从这点可以想到

$$ilde{w} = egin{bmatrix} w \ \sqrt{2C} \xi_1 \ \dots \ \sqrt{2C} \xi_N \end{bmatrix}$$

从而

$$ilde{w}^T ilde{w}=w^Tw+2C\sum_{n=1}^N \xi_n^2$$

这样变换之后也要对条件进行变换,将条件化为 $y_n(w^T \tilde{x}_n + b) \geq 1$ 的形式

$$egin{aligned} y_n(w^Tx_n+b) &\geq 1-\xi_n \Leftrightarrow \ y_n(w^Tx_n+b+y_n\xi_n) &\geq 1 \Leftrightarrow \ y_n(w^Tx_n+\sqrt{2C}\xi_n(rac{1}{\sqrt{2C}}y_n)+b) &\geq 1 \end{aligned}$$

结合 $ilde{w}$ 的式子,我们可以定义 $ilde{x}_n$,注意 $x_n \in \mathbb{R}^k$

$$ilde{x}_n = \left[egin{array}{c} x_n \ 0 \ \dots \ rac{1}{\sqrt{2C}} y_n \ \dots \ 0 \end{array}
ight] \in \mathbb{R}^{k+N}$$

其中 $ilde{x}_n$ 的第k+1到k+N的分量中,除了第k+n个为 $\frac{1}{\sqrt{2C}}y_n$,其余均为0,这样就把问题转化为

$$\min_{w,b,\xi} \ rac{1}{2} ilde{w}^T ilde{w}$$
 subject to $y_n(ilde{w}^T x_n + b) \geq 1$

如果已经计算出了 \tilde{w} ,那么由于

$$ilde{w} = egin{bmatrix} w \ \sqrt{2C} \xi_1 \ \dots \ \sqrt{2C} \xi_N \end{bmatrix}$$

所以取 w的前k个分量即可得到w。

Problem 12

只要看这些映射对应的Gram矩阵是否半正定即可,设 K,K_1,K_2 对应的Gram矩阵为 M,M_1,M_2 (a) $K(x,x^{'})=K_1(x,x^{'})+K_2(x,x^{'})$ 可得 $M=M_1+M_2$

$$y^T M y = y^T (M_1 + M_2) y = y^T M_1 y + y^T M_2 y \geq 0$$

所以 $K(x,x^{'})=K_{1}(x,x^{'})+K_{2}(x,x^{'})$ 为kernerl

(b)
$$K(x,x^{'})=K_{1}(x,x^{'})-K_{2}(x,x^{'})$$
可得 $M=M_{1}-M_{2}$

这个一看就不是kernel, 反例也很好构造

$$M_1=egin{bmatrix}1&0\0&1\end{bmatrix}, M_2=egin{bmatrix}2&0\0&2\end{bmatrix}, M=M_1-M_2=egin{bmatrix}-1&0\0&-1\end{bmatrix}$$

显然M不是半正定的,所以 $K(x,x^{'})=K_{1}(x,x^{'})-K_{2}(x,x^{'})$ 不是kernel (c)首先计算下式子的形式。

$$egin{aligned} K(x,x^{'}) &= K_{1}(x,x^{'})K_{2}(x,x^{'}) = \phi_{1}(x)^{T}\phi_{1}(x^{'})\phi_{2}(x)^{T}\phi_{2}(x^{'}) \ &= \sum_{i=1}^{n}\phi_{1}^{i}(x)\phi_{1}^{i}(x^{'})\sum_{j=1}^{n}\phi_{2}^{j}(x)\phi_{2}^{j}(x^{'}) \ &= \sum_{i=1}^{n}\sum_{j=1}^{n}\phi_{1}^{i}(x)\phi_{1}^{i}(x^{'})\phi_{2}^{j}(x)\phi_{2}^{j}(x^{'}) \ &= \sum_{i=1}^{n}\sum_{j=1}^{n}(\phi_{1}^{i}(x)\phi_{2}^{j}(x))(\phi_{1}^{i}(x^{'})\phi_{2}^{j}(x^{'})) \end{aligned}$$

根据这个形式,可以做以下定义

$$\Phi^i(x) = \phi^i_1(x)(\phi^1_2(x), \dots, \phi^n_2(x)) \ \Phi(x) = (\Phi^1(x), \dots, \Phi^n(x))^T$$

我们来计算下这个式子

$$(\Phi^{i}(x))^{T}(\Phi^{i}(x^{'})) = \sum_{j=1}^{n} (\phi_{1}^{i}(x)\phi_{2}^{j}(x))(\phi_{1}^{i}(x^{'})\phi_{2}^{j}(x^{'})) \ (\Phi(x))^{T}\Phi(x^{'}) = \sum_{i=1}^{n} (\Phi^{i}(x))^{T}(\Phi^{i}(x^{'})) = \sum_{i=1}^{n} \sum_{j=1}^{n} (\phi_{1}^{i}(x)\phi_{2}^{j}(x))(\phi_{1}^{i}(x^{'})\phi_{2}^{j}(x^{'})) = K(x,x^{'})$$

根据核函数的定义可知, $K(x,x^{'})=K_1(x,x^{'})K_2(x,x^{'})$ 为kernel $(d)K(x,x^{'})=K_1(x,x^{'})/K_2(x,x^{'})$

这个也不是kernel, 反例如下

$$M_1=egin{bmatrix}1&2\2&3\end{bmatrix}, M_2=egin{bmatrix}2&1\1&1\end{bmatrix}, M=M_1/M_2=egin{bmatrix}rac12&2\2&3\end{bmatrix}$$

M行列式小于0,所以必然不是半正定的,所以 $K(x,x^{'})=K_{1}(x,x^{'})/K_{2}(x,x^{'})$ 不是kernel 所以这题答案为(a)(c)。

Problem 13

设 K, K_1 对应的Gram矩阵为 M, M_1

(a)

$$M_1 = egin{bmatrix} 1 & 0 \ 0 & 1 \end{bmatrix}, M = egin{bmatrix} (1-1)^2 & (1-0)^2 \ (1-0)^2 & (1-1)^2 \end{bmatrix} = egin{bmatrix} 0 & 1 \ 1 & 0 \end{bmatrix}$$

M的行列式小于0,所以 $K(x,x^{'})=(1-K_{1}(x,x^{'}))^{2}$ 不是kernel

(b)

$$M = 1126M_1$$

因为 M_1 半正定,所以M半正定,从而 $K(x,x^{'})=1126K_1(x,x^{'})$ 是kernel (c)

$$M_1 = egin{bmatrix} 1 & 0 \ 0 & 1 \end{bmatrix}, M = egin{bmatrix} e^{-1} & 1 \ 1 & e^{-1} \end{bmatrix}$$

M的行列式小于0,所以 $K(x,x^{'})=\exp(-K_{1}(x,x^{'}))$ 不是kernel (d)利用 $f(x)=rac{1}{1-x}$ 在(0,1)区间的泰勒展开可得

$$egin{aligned} K(x,x^{'}) &= (1-K_{1}(x,x^{'}))^{-1} \ &= \sum_{i=0}^{+\infty} (K_{1}(x,x^{'}))^{i} \end{aligned}$$

由上题的(b)我们知道 $K_1(x,x^{'})^i$ 为kernel,再有上题的(a)我们知道kernel的和也为kernel,所以

$$K(x,x^{'})=\sum_{i=0}^{+\infty}(K_{1}(x,x^{'}))^{i}$$

也为kernel

Problem 14

首先回顾下对偶问题对应的QP问题

$$egin{aligned} \min & \min_{lpha \in R^N} : rac{1}{2}lpha^T Q_Dlpha - 1_N^Tlpha \ & ext{subject to: } A_Dlpha \geq u \end{aligned} \ Q_D = egin{bmatrix} y_1y_1K_{11} & \dots & y_1y_NK_{1N} \ y_2y_1K_{12} & \dots & y_2y_NK_{2N} \ \dots & \dots & \dots \ y_Ny_1K_{N1} & \dots & y_Ny_NK_{NN} \end{bmatrix}, A_D = egin{bmatrix} y^T \ -y^T \ I_{N imes N} \ -I_{N imes N} \end{bmatrix}, u = egin{bmatrix} 0 \ 0 \ 0 \ 0_{N imes N} \ C imes I_{N imes N} \end{bmatrix} \end{aligned}$$

我们来看如果用新的kernel, $ilde{K}(x,x^{'})=pK(x,x^{'})+q$,并且 $ilde{C}=rac{C}{p}$ 会产生什么情况:

接着我们来计算 $\alpha^T \tilde{Q}_D \alpha$, 注意

$$(y_1,\ldots,y_N)$$
. $\alpha=0$

所以

$$lpha^T ilde{Q}_D lpha = lpha^T p Q_D lpha + lpha^T q(y_1, \ldots, y_N)^T (y_1, \ldots, y_N) lpha = p lpha^T Q_D lpha$$

所以我们的目标函数为

$$rac{1}{2}lpha^T ilde{Q}_Dlpha-1_N^Tlpha=rac{1}{2}plpha^T ilde{Q}_Dlpha-1_N^Tlpha=rac{1}{p}[rac{1}{2}(plpha)^TQ_D(plpha)-1_N^T(plpha)]$$

由于p为常数, 所以目标函数可以简化为

$$rac{1}{2}(plpha)^TQ_D(plpha)-1_N^T(plpha)$$

再看下限制条件

$$ilde{A}_Dlpha \geq ilde{u} \Leftrightarrow A_Dlpha \geq rac{1}{p}u \Leftrightarrow A_D(plpha) \geq u$$

我们令 $\overline{\alpha} = p\alpha$,那么问题可以转换为

$$\begin{aligned} & \underset{\alpha \in R^N}{\text{minimize}} : \frac{1}{2}\overline{\alpha}^T Q_D \overline{\alpha} - 1_N^T \overline{\alpha} \\ & \text{subject to: } A_D \overline{\alpha} \geq u \end{aligned} \\ Q_D = \begin{bmatrix} y_1 y_1 K_{11} & \dots & y_1 y_N K_{1N} \\ y_2 y_1 K_{12} & \dots & y_2 y_N K_{2N} \\ \dots & \dots & \dots \\ y_N y_1 K_{N1} & \dots & y_N y_N K_{NN} \end{bmatrix}, A_D = \begin{bmatrix} y^T \\ -y^T \\ I_{N \times N} \\ -I_{N \times N} \end{bmatrix}, u = \begin{bmatrix} 0 \\ 0 \\ 0_{N \times N} \\ C \times I_{N \times N} \end{bmatrix}$$

可以看出,这个问题和原问题是一致的,记原问题的最优解为 $lpha^*$,那么该问题的最优解 $ilde{lpha}^*$ 满足以下条件

$$\alpha^* = p\tilde{\alpha}^*$$

我们根据这个条件开始讨论问题。

回顾下soft-margin得到的计算公式

如果我们将kernel换成

$$ilde{K}(x,x^{'})=pK(x,x^{'})+q$$

利用之前的条件 $lpha^*=p ilde{lpha}^*$ 以及 $ilde{C}=rac{C}{p},\sum_{n=1}^Nlpha_n^*y_n=0$,可以对变换kernel之后的问题求解

$$egin{aligned} ilde{w}^* &= \sum_{n=1}^N ilde{lpha}_n^* y_n z_n = rac{1}{p} (\sum_{n=1}^N lpha_n^* y_n z_n) = rac{w^*}{p} \ ilde{eta}_n^* &= ilde{C} - ilde{lpha}_n^* = rac{C}{p} - rac{lpha_n^*}{p} = rac{1}{p} (C - lpha_n^*) = rac{eta_n}{p} (n = 1, \dots, N) \end{aligned}$$

$$egin{aligned} ilde{b}^* &= y_m - \sum_{n=1}^N ilde{lpha}_n^* y_n ilde{K}(x_n, x_m) \ &= y_m - \sum_{n=1}^N rac{lpha_n^*}{p} y_n (pK(x_n, x_m) + q) \ &= y_m - \sum_{n=1}^N lpha_n^* y_n K(x_n, x_m) - rac{q}{p} \sum_{n=1}^N lpha_n^* y_n \ &= y_m - \sum_{n=1}^N lpha_n^* y_n K(x_n, x_m) \ &= b^* \end{aligned}$$

$$egin{aligned} ilde{g}(x) &= ext{sign}(\sum_{n=1}^{N} ilde{lpha}_{n}^{*}y_{n} ilde{K}(x_{n},x) + ilde{b}^{*}) \ &= ext{sign}[\sum_{n=1}^{N} rac{lpha_{n}^{*}}{p}y_{n}(pK(x_{n},x) + q) + b^{*}] \ &= ext{sign}[\sum_{n=1}^{N} lpha_{n}^{*}y_{n}K(x_{n},x) + rac{q}{p}\sum_{n=1}^{N} lpha_{n}^{*}y_{n} + b^{*}] \ &= ext{sign}(\sum_{n=1}^{N} lpha_{n}^{*}y_{n}K(x_{n},x) + b^{*}) \ &= g(x) \end{aligned}$$

这说明这样变换之后我们的分类器没有变。

Problem 15

首先读取数据并作图

```
# -*- coding: utf-8 -*-
"""
Created on Wed Mar 27 13:42:18 2019

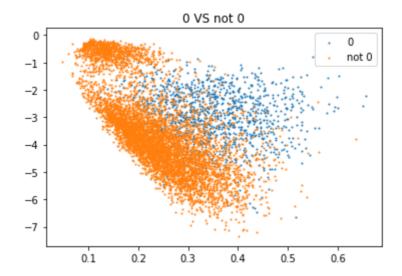
@author: qinzhen
"""

####Problem 15
import matplotlib.pyplot as plt
import numpy as np
from sklearn import svm

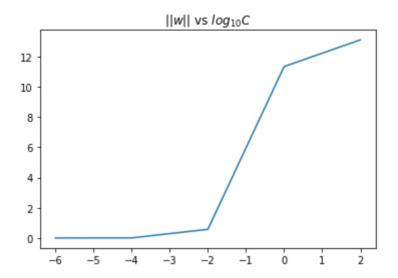
def transformdata(file):
    data = np.genfromtxt(file)
    y, X = data[:, 0], data[:, 1:]
    return X, y
```

```
train = "featurestrain.txt"
X_train, y_train = transformdata(train)
test = "featurestest.txt"
X_test,y_test = transformdata(test)

#作图
plt.scatter(X_train[y_train == 0][:, 0], X_train[y_train == 0][:, 1], s=1, label='0')
plt.scatter(X_train[y_train != 0][:, 0], X_train[y_train != 0][:, 1], s=1, label='not 0')
plt.title('0 vs not 0')
plt.legend()
plt.show()
```

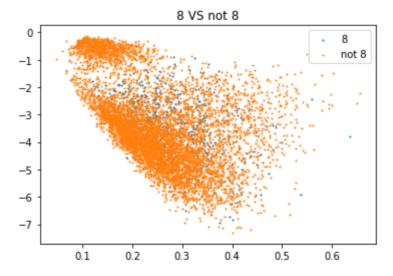


接着训练模型并作图:



注意这题是8和not 8, 首先作图

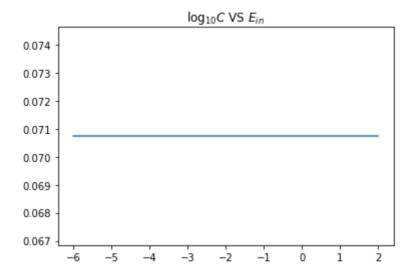
```
####Problem 16
plt.scatter(X_train[y_train == 8][:, 0], X_train[y_train == 8][:, 1], s=1, label='8')
plt.scatter(X_train[y_train != 8][:, 0], X_train[y_train != 8][:, 1], s=1, label='not 8')
plt.title('8 VS not 8')
plt.legend()
plt.show()
```



注意17题要计算 $\sum_{n=1}^N \alpha_n$,所以我们这题把系数也算出来,由于sklearn只能计算对偶系数 $y_n\alpha_n$,所以这里要把标签转换为+1,-1,方便计算。

```
#训练
y_train_8 = 2 * (y_train==8).astype("int") - 1
C = [-6, -4, -2, 0, 2]
Ein = []
alpha = []
for i in C:
```

```
c = 10 ** iclf = svm.SVC(kernel='poly', degree=2, coef0=1, gamma=1, C=c)clf.fit(X_train, y_train_8)e = np.mean(clf.predict(X_train) != y_train_8)#支持向量的索引support = clf.support_#计算系数coef = np.sum(clf.dual_coef_[0] * y_train_8[support])alpha.append(coef)Ein.append(e)
#作图
plt.plot(C,Ein)
plt.show()
```

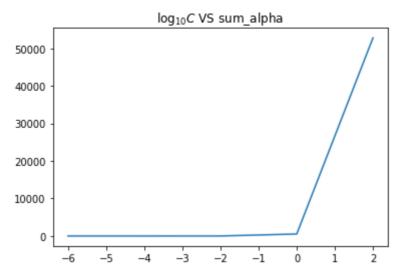


比较神奇的是这题的Ein都一样。

Problem 17

利用上题的数据作图即可。

```
####Problem 17
plt.plot(C, alpha)
plt.title("$\log_{10}C$ VS sum_alpha")
plt.show()
```



可以看到尽管上题的 E_{in} 一致,但是这里 $\sum_{n=1}^{N} \alpha_n$ 会增加。

Problem 18

这题需要计算权重w, 因为涉及到高斯核, 无法直接计算。

现在假设有n个样本,那么:

$$egin{aligned} w &= \sum_{i=1}^n lpha_i y_i z_i, z_i = \Phi\left(x_i
ight) \ \|w\|^2 &= \sum_{i=1}^n \sum_{j=1}^n lpha_i y_i lpha_j y_j z_i^T z_j = \sum_{i=1}^n \sum_{j=1}^n lpha_i y_i lpha_j y_j z_i^T z_j K\left(x_i, x_j
ight) \end{aligned}$$

其中

$$K(x_i,x_j) = \exp\Bigl(-\gamma ||x_i-x_j||^2\Bigr)$$

记

$$ar{y} = egin{bmatrix} lpha_1 y_1 \ dots \ lpha_n y_n \end{bmatrix} \in \mathbb{R}^n, D \in \mathbb{R}^{n imes n}, D_{ij} = \left|\left|x_i - x_j
ight|
ight|^2$$

那么

$$K = \exp(-\gamma D)$$

并且

$$\|w\|^2 = ar{y}^T K ar{y}$$

注意只有支持向量部分的系数非零,所以上述计算步骤只要对支持向量进行即可 (clf.support_为支持向量的索引) ,所以只要计算出D即可,这里介绍向量化的计算方法,考虑更一般的问题:

假设

$$X = egin{bmatrix} -(x^{(1)})^T - \ -(x^{(2)})^T - \ dots \ -(x^{(m)})^T - \end{bmatrix} \in \mathbb{R}^{m imes d}, Y = egin{bmatrix} -(y^{(1)})^T - \ -(y^{(2)})^T - \ dots \ -(y^{(n)})^T - \end{bmatrix} \in \mathbb{R}^{n imes d}$$

其中 $x^{(i)},y^{(i)}\in\mathbb{R}^d$,现在的问题是如何高效计算矩阵 $D\in\mathbb{R}^{m imes n}$,其中

$$D_{i,j} = ||x^{(i)} - y^{(j)}||^2$$

首先对 $D_{i,j}$ 进行处理

$$egin{aligned} D_{i,j} &= ||x^{(i)} - y^{(j)}||^2 \ &= (x^{(i)} - y^{(j)})^T (x^{(i)} - y^{(j)}) \ &= (x^{(i)})^T x^{(i)} - 2 (x^{(i)})^T y^{(j)} + (y^{(j)})^T y^{(j)} \end{aligned}$$

那么

$$\begin{split} D &= \begin{bmatrix} D_{1,1} & \dots & D_{1,n} \\ \dots & \dots & \dots \\ D_{m,1} & \dots & D_{m,n} \end{bmatrix} \\ &= \begin{bmatrix} (x^{(1)})^T x^{(1)} - 2(x^{(1)})^T y^{(1)} + (y^{(1)})^T y^{(1)} & \dots & (x^{(1)})^T x^{(1)} - 2(x^{(1)})^T y^{(n)} + (y^{(n)})^T y^{(n)} \\ \dots & \dots & \dots & \dots \\ (x^{(m)})^T x^{(m)} - 2(x^{(m)})^T y^{(1)} + (y^{(1)})^T y^{(1)} & \dots & (x^{(m)})^T x^{(m)} - 2(x^{(m)})^T y^{(n)} + (y^{(n)})^T y^{(n)} \end{bmatrix} \\ &= \begin{bmatrix} (x^{(1)})^T x^{(1)} & \dots & (x^{(1)})^T x^{(1)} \\ \dots & \dots & \dots \\ (x^{(m)})^T x^{(m)} & \dots & (x^{(m)})^T x^{(m)} \end{bmatrix} + \begin{bmatrix} (y^{(1)})^T y^{(1)} & \dots & (y^{(n)})^T y^{(n)} \\ \dots & \dots & \dots \\ (y^{(n)})^T y^{(n)} \end{bmatrix} - 2 \begin{bmatrix} (x^{(1)})^T y^{(1)} & \dots & (x^{(m)})^T y^{(n)} \\ \dots & \dots & \dots \\ (x^{(m)})^T y^{(1)} & \dots & (x^{(m)})^T y^{(n)} \end{bmatrix} \\ &= \begin{bmatrix} (x^{(1)})^T x^{(1)} \\ \dots \\ (x^{(m)})^T x^{(m)} \end{bmatrix} \underbrace{ \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}}_{1 \times n \not \bowtie p} + \underbrace{ \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{m \times 1 \not \bowtie p} \begin{bmatrix} (y^{(1)})^T y^{(1)} & \dots & (y^{(n)})^T y^{(n)} \end{bmatrix} - 2XY^T \end{split}$$

利用numpy的广播机制上式可以简写如下:

```
#計算距离矩阵

d1 = np.sum(X ** 2, axis=1).reshape(-1, 1)

d2 = np.sum(Y ** 2, axis=1).reshape(1, -1)

dist = d1 + d2 - 2 * X.dot(Y.T)
```

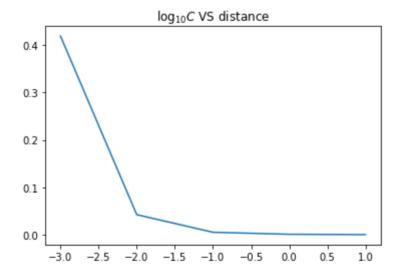
利用上述方法计算 $\|w\|^2$ 即可,最后注意距离为 $\frac{1}{\|w\|^2}$:

```
####Problem 18

C = [-3, -2, -1, 0, 1]

Distance = []
```

```
#将标签修改为-1,1
y = 2 * y_train_1 - 1
for i in C:
   c = 10**i
    clf = svm.SVC(kernel='rbf', gamma=1, C=c)
   clf.fit(X_train, y)
   X = X_train[clf.support_]
   #距离矩阵
   d1 = np.sum(x ** 2, axis=1).reshape(-1, 1)
   d2 = np.sum(X ** 2, axis=1).reshape(1, -1)
   dist = d1 + d2 - 2 * X.dot(X.T)
   #Kernel矩阵
    K = np.exp(-c * dist)
   #计算anyn
   y1 = clf.dual_coef_[0] * y[clf.support_]
   w2 = y1.dot(K).dot(y1.T)
   #计算距离
    distance = 1 / np.sqrt(w2)
    Distance.append(distance)
plt.plot(C, Distance)
plt.title("$\log_{10}C$ VS distance")
plt.show()
```



随着C增加,距离在减少。

Problem 19

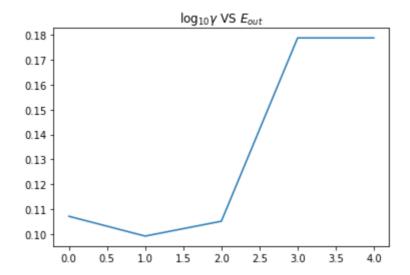
```
####Problem 19
y_test_1 = (y_test == 0)

Gamma = range(5)
Eout = []

for i in Gamma:
```

```
gamma = 10**i
  clf = svm.SVC(kernel='rbf', gamma=gamma, C=0.1)
  clf.fit(X_train, y_train_1)
  e = np.mean(clf.predict(X_test) != y_test_1)
  Eout.append(e)

plt.plot(Gamma, Eout)
plt.title("$\log_{10}\gamma$ \sum \$E_{out}$")
plt.show()
```



可以看到, $\log_{10}\gamma=1$ 时, E_{out} 最小, 说明C不能太大, 也不能太小。

这题要构造交叉验证集,多次实验,做直方图,先做一些预处理。

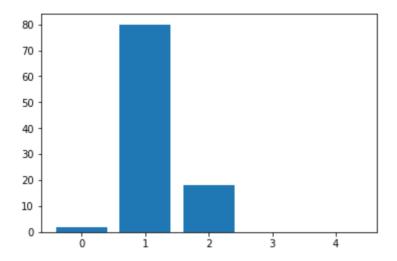
```
####Problem 20
from sklearn.model_selection import train_test_split
#对数据合并,方便调用train_test_split函数
Data = np.c_[X_train, y_train]
N = 100
#记录最小Eval对应的gamma的索引的次数
Cnt = np.zeros(5)
Gamma = range(5)
for _ in range(N):
   #划分数据
   train_set, val_set = train_test_split(Data, test_size=0.2)
   #取特征
   X_train = train_set[:, :2]
   #取标签
   y_train = train_set[:, 2]
   X_val = val_set[:, :2]
   y_val = val_set[:, 2]
   Eval = []
```

```
for i in Gamma:
    gamma = 10 ** i
    clf = svm.SVC(kernel='rbf', gamma=gamma, C=0.1)
    clf.fit(X_train, y_train)
    e = np.mean(clf.predict(X_val) != y_val)
    Eval.append(e)

#找到最小Eval对应的索引
index = np.argmin(Eval)

#对应索引次数加1
Cnt[index] += 1

plt.bar(Gamma, Cnt)
plt.show()
```



可以看到大部分最优解对应的 $\log_{10}\gamma$ 都为1,和上一题说明同一个道理,说明 γ 不能太大,也不能太小。

附加题

Problem 21

这题的问题是求hard-margin SVM对偶问题的对偶问题,我们来看一下。

首先回顾下hard-margin SVM对偶问题。

$$egin{aligned} & ext{minimize}: rac{1}{2} \sum_{m=1}^N \sum_{n=1}^N y_n y_m lpha_n lpha_m x_n^T x_m - \sum_{n=1}^N lpha_n \ & ext{subject to:} \ \sum_{n=1}^N y_n lpha_n = 0, lpha_n \geq 0 (n=1,\ldots,N) \end{aligned}$$

根据拉格朗日乘子法, 我们将上述问题转化为

$$\min_{lpha \in \mathbb{R}^N} \max_{\lambda_i \geq 0} : rac{1}{2} \sum_{m=1}^N \sum_{n=1}^N y_n y_m lpha_n lpha_m x_n^T x_m - \sum_{n=1}^N lpha_n + \lambda_0 (\sum_{n=1}^N y_n lpha_n) - \sum_{n=1}^N \lambda_n lpha_n$$

min max = max min

所以上述问题可以转化为

$$\max_{\lambda_i \geq 0} \min_{lpha \in \mathbb{R}^N} : rac{1}{2} \sum_{m=1}^N \sum_{n=1}^N y_n y_m lpha_n lpha_m x_n^T x_m - \sum_{n=1}^N lpha_n + \lambda_0 (\sum_{n=1}^N y_n lpha_n) - \sum_{n=1}^N \lambda_n lpha_n$$

这个最小值问题转化为为一个无条件极值,现在做以下记号

$$f(\lambda,lpha) = rac{1}{2}\sum_{m=1}^N\sum_{n=1}^N y_n y_m lpha_n lpha_m x_n^T x_m - \sum_{n=1}^N lpha_n + \lambda_0 (\sum_{n=1}^N y_n lpha_n) - \sum_{n=1}^N \lambda_n lpha_n$$

关于 α_i 求偏导可得

$$egin{aligned} rac{\partial f}{\partial lpha_i} &= rac{1}{2} \sum_{n=1}^N y_n y_i lpha_n x_n^T x_i + rac{1}{2} \sum_{m=1}^N y_i y_m lpha_m x_i^T x_m - 1 + \lambda_0 y_i - \lambda_i \ &= \sum_{n=1}^N y_n y_i lpha_n x_i^T x_n - 1 + \lambda_0 y_i - \lambda_i \end{aligned}$$

令偏导为0可得

$$\sum_{n=1}^N y_n y_i lpha_n x_i^T x_n = 1 - \lambda_0 y_i + \lambda_i$$

对这个式子作以下变形可得

$$\left[egin{array}{cccc} y_i y_1 x_i^T x_1 & \dots & y_i y_N x_i^T x_N \end{array}
ight] \left[egin{array}{c} lpha_1 \ \dots \ lpha_N \end{array}
ight] = 1 - \lambda_0 y_i + \lambda_i \end{array}$$

这个形式是见过的,我们回顾下Learning from data第八章的28页,我们知道hard-margin SVM对偶问题也可以写成如下的形式

$$egin{aligned} & & & \min & \sum_{lpha \in \mathbb{R}^N} : rac{1}{2} lpha^T Q_D lpha - \mathbf{1}_N^T lpha \ & & ext{subject to: } A_D lpha \geq 0_{N+2} \ Q_D = egin{bmatrix} y_1 y_1 x_1^T x_1 & \dots & y_1 y_N x_1^T x_N \ y_2 y_1 x_2^T x_1 & \dots & y_2 y_N x_2^T x_N \ \dots & \dots & \dots \ y_N y_1 x_N^T x_1 & \dots & y_N y_N x_N^T x_N \end{bmatrix} ext{ and } A_D = egin{bmatrix} y^T \ -y^T \ I_{N imes N} \end{bmatrix} \end{aligned}$$

(1)的等式左边的第一个向量对应着 Q_D 的每一行,所以如果我们对(1)式中i从1取到N,可以把(1)的条件转化为

$$Q_Dlpha = 1_N - \lambda_0 y + \lambda \ lpha = egin{bmatrix} lpha_1 \ lpha_N \end{bmatrix}, y = egin{bmatrix} y_1 \ lpha_N \end{bmatrix}, \lambda = egin{bmatrix} \lambda_1 \ lpha \ lpha_N \end{bmatrix}$$

在这个记号下, 对原问题进行处理

$$egin{aligned} \sum_{m=1}^{N}\sum_{n=1}^{N}y_{n}y_{m}lpha_{n}lpha_{m}x_{n}^{T}x_{m} &= lpha^{T}Q_{D}lpha \ &\sum_{n=1}^{N}lpha_{n} &= 1_{N}^{T}lpha \ &\lambda_{0}(\sum_{n=1}^{N}y_{n}lpha_{n}) &= \lambda_{0}lpha^{T}y \ &\sum_{n=1}^{N}\lambda_{n}lpha_{n} &= lpha^{T}\lambda \end{aligned}$$

所以

$$f(\lambda, lpha) = rac{1}{2} lpha^T Q_D lpha - \mathbb{1}_N^T lpha + \lambda_0 lpha^T y - lpha^T \lambda$$

将 $Q_D \alpha = 1_N - \lambda_0 y + \lambda$ 带入可得

$$egin{aligned} f(\lambda,lpha) &= rac{1}{2}lpha^TQ_Dlpha - \mathbb{1}_N^Tlpha + \lambda_0lpha^Ty - lpha^T\lambda \ &= rac{1}{2}lpha^T(\mathbb{1}_N - \lambda_0y + \lambda) - \mathbb{1}_N^Tlpha + \lambda_0lpha^Ty - lpha^T\lambda \ &= -rac{1}{2}lpha^T\mathbb{1}_N + rac{1}{2}\lambda_0lpha^Ty - rac{1}{2}lpha^T\lambda \ &= -rac{1}{2}lpha^T(\mathbb{1}_N - \lambda_0y + \lambda) \end{aligned}$$

如果 Q_D 可逆,那么

$$lpha = Q_D^{-1}(1_N - \lambda_0 y + \lambda)$$

代入可得

$$egin{aligned} -rac{1}{2}lpha^T(1_N-\lambda_0 y+\lambda) &= -rac{1}{2}[Q_D^{-1}(1_N-\lambda_0 y+\lambda)]^T(1_N-\lambda_0 y+\lambda) \ &= -rac{1}{2}(1_N-\lambda_0 y+\lambda)^TQ_D^{-1}(1_N-\lambda_0 y+\lambda) \end{aligned}$$

所以问题转化为

$$egin{aligned} & ext{maxmize}: -rac{1}{2}(1_N - \lambda_0 y + \lambda)^T Q_D^{-1}(1_N - \lambda_0 y + \lambda) \ & ext{subject to: } \lambda_i \geq 0 (n = 0, 1, \dots, N) \end{aligned}$$

把负号提出来,可以转化为标准的QP问题

$$egin{aligned} & \operatornamewithlimits{minmize}_{\lambda_i \geq 0} : rac{1}{2} (1_N - \lambda_0 y + \lambda)^T Q_D^{-1} (1_N - \lambda_0 y + \lambda) \ & ext{subject to: } \lambda_i \geq 0 (n = 0, 1, \dots, N) \end{aligned}$$

可以看到,这和最开始的问题是非常类似的。