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

$$\begin{aligned} \min_{w,b,\xi} \quad & \frac{1}{2}w^Tw + C\sum_{n=1}^{N}\xi_n \\ \text{subject to} \quad & y_n(w^Tx_n + b) \geq 1 - \xi_n \\ & \xi_n \geq 0 (n = 1, \dots, N) \end{aligned}$$

除了x_n, y_n，其余量均为参数，注意$w \in \mathbb{R}^d$，所以我们的参数有

$$w = (w_1, \dots, w_d), \xi_1, \dots, \xi_N, C$$

一共$d + N + 1$个。限制条件为

$$\begin{aligned} & y_n(w^Tx_n + b) \geq 1 - \xi_n \\ & \xi_n \geq 0 (n = 1, \dots, N) \end{aligned}$$

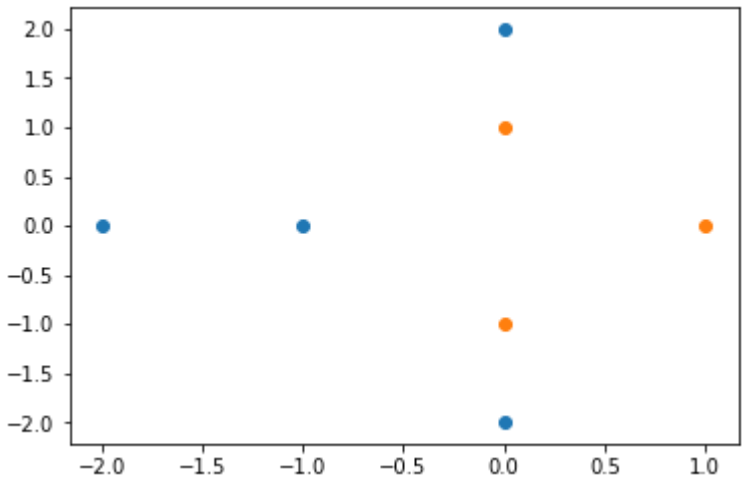
一共有$2N$个。

Problem 2

首先作图看下

```
import numpy as np
import matplotlib.pyplot as plt

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,+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

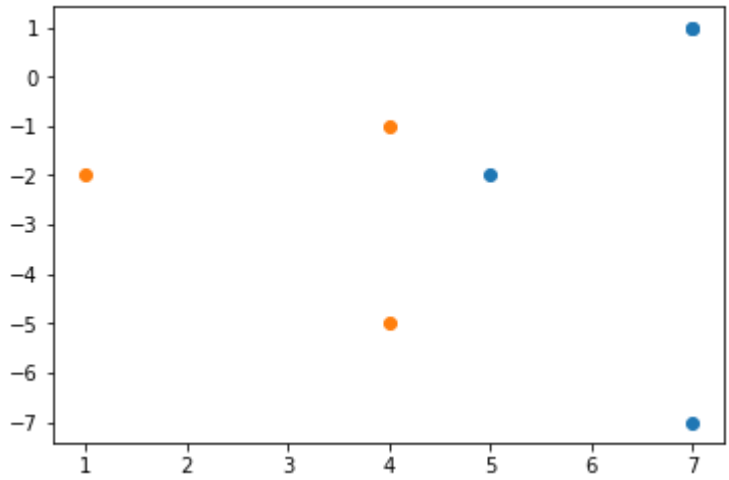
$$z_4 = (5, -2), z_5 = (7, -7), z_6 = (7, 1), z_7 = (7, 1)$$

转换之后的标记为$+1$的点为

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

```
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 = []
for i in x:
    X.append([phi_1(i),phi_2(i)])
X = np.array(X)

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()
```

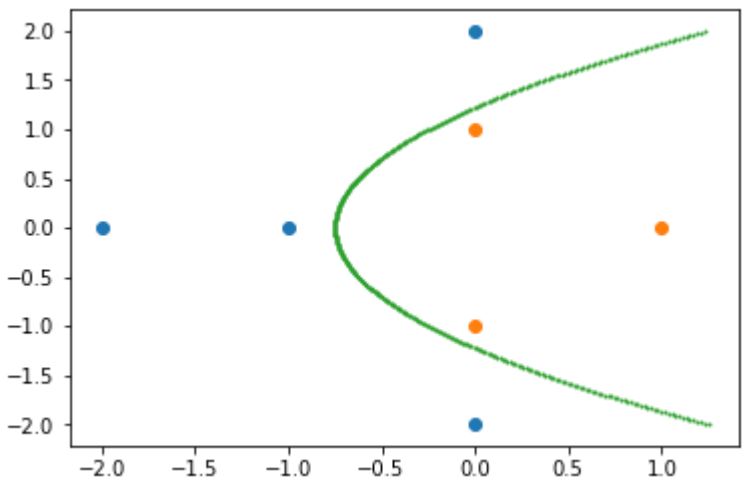


从这个图像中可以看出，最大间隔分类器为$\varphi_1(x)=4.5$，将$\varphi_1(x)=x_2^2-2x_1+3$带入可得最大间隔分类器为

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

最后看下曲线的图。

```
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()
```



Problem 3

利用sklearn处理即可。

```
from sklearn import svm

clf = svm.SVC(kernel='poly',degree=2,coef0=1,gamma=1,C=1e10)
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=True,
  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([[-0.59647182, -0.81065085,  0.8887034 ,  0.20566488,  0.31275439]])
```

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([ 0.59647182,  0.81065085,  0.8887034 ,  0.20566488,  0.31275439])
```

所以

$$(\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5,\alpha_6,\alpha_7)=(0,0.59647182,0.81065085,0.8887034,0.20566488,0.31275439,0)$$

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

$$b^* = y_s - \sum_{\alpha_n^*>0} y_n \alpha_n^* z_n^T z_s$$

$$g(x) = \text{sign}(\sum_{n=1}^{N} y_n \alpha_n^* z_n^T z + b^*)$$

$$z = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$$

利用这两个式子计算即可。

```
def g(x):
    r = np.sqrt(2)
    return np.array([1,r*x[0],r*x[1],x[0]**2,x[0]*x[1],x[1]*x[0],x[1]**2])

support = clf.support_
coef = clf.dual_coef_[0]
x4 = np.array([g(i) for i in x])

#取第一个支持向量
s = support[0]

b = z[s] - coef.dot(x4[support].dot(x4[s]))
k = (coef).dot(x4[support])

b,k
```

```
(-1.6665544170710518,
 array([ -5.55111512e-17,  -1.25681640e+00,   1.11022302e-16,
          8.88703402e-01,   0.00000000e+00,   0.00000000e+00,
          6.66554417e-01]))
```

所以曲线方程为

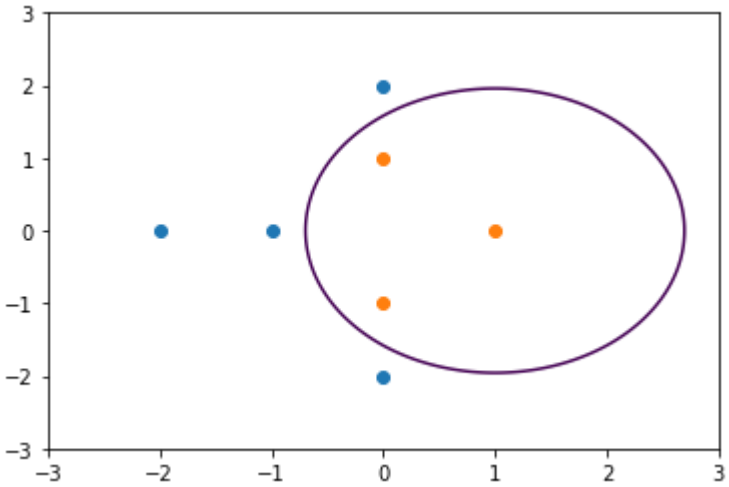
$$k^T z + b = 0$$

Problem 5

我们来作图，利用等高线的技巧。

```
#构造等高线函数
def g(x,y,k,b):
    r = np.sqrt(2)
    return k[0]+k[1]*r*x+k[2]*r*y+k[3]*(x**2)+(k[4]+k[5])*x*y+k[6]*(y**2)+b

#点的数量
n = 1000
r = 3

#作点
```

```
p = np.linspace(-r,r,n)
q = np.linspace(-r,r,n)

#构造网格
P,Q = np.meshgrid(p,q)

#绘制等高线
plt.contour(P,Q,g(P,Q,k,b),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

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

所以在$||x_n - c||^2 \leq R^2$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

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

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

$$\begin{aligned}c\sum_{n=1}^N\lambda_n-\sum_{n=1}^N\lambda_nx_n&=0\\c&=\frac{\sum_{n=1}^N\lambda_nx_n}{\sum_{n=1}^N\lambda_n}\end{aligned}$$

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

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

$$c=\frac{\sum_{n=1}^N\lambda_nx_n}{\sum_{n=1}^N\lambda_n}=\sum_{n=1}^N\lambda_nx_n$$

Problem 8

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

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

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

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

再带入$c = \sum_{n=1}^{N}\lambda_nx_n$

$$
\begin{aligned}
L(R,c,\lambda) &= \sum_{n=1}^{N}\lambda_nx_n^Tx_n - 2c\sum_{n=1}^{N}\lambda_nx_n^T + c^Tc \\
&= \sum_{n=1}^{N}\lambda_nx_n^Tx_n - 2(\sum_{n=1}^{N}\lambda_nx_n^T)(\sum_{n=1}^{N}\lambda_nx_n) + (\sum_{n=1}^{N}\lambda_nx_n^T)(\sum_{n=1}^{N}\lambda_nx_n) \\
&= \sum_{n=1}^{N}\lambda_nx_n^Tx_n - (\sum_{n=1}^{N}\lambda_nx_n^T)(\sum_{n=1}^{N}\lambda_nx_n)
\end{aligned}
$$

所以问题转换为

$$
\begin{aligned}
&\text{在条件}\sum_{n=1}^{N}\lambda_n = 1, \lambda_n \geq 0\text{下}, \\
&\text{最小化}f(\lambda) = \sum_{n=1}^{N}\lambda_nx_n^Tx_n - (\sum_{n=1}^{N}\lambda_nx_n^T)(\sum_{n=1}^{N}\lambda_nx_n)
\end{aligned}
$$

Problem 9

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

$$
\begin{aligned}
f(\lambda) &= \sum_{n=1}^{N}\lambda_nx_n^Tx_n - (\sum_{n=1}^{N}\lambda_nx_n^T)(\sum_{n=1}^{N}\lambda_nx_n) \\
&= \sum_{n=1}^{N}\lambda_nx_n^Tx_n - \sum_{n=1}^{N}\sum_{m=1}^{N}\lambda_n\lambda_mx_n^Tx_m
\end{aligned}
$$

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

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

Problem 10

由Problem 6的推导过程我们可知，

$$
\begin{gathered}
\lambda_n(||x_n - c||^2 - R^2) = 0 \\
n = 1, \dots, N
\end{gathered}
$$

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

$$
\begin{gathered}
\lambda_n(||z_n - c||^2 - R^2) = 0 \\
n = 1, \dots, N
\end{gathered}
$$

所以如果存在$\lambda_i \neq 0$，那么

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

结合$c = \sum_{n=1}^{N} \lambda_n z_n$，就能计算出$R$了

Problem 11

首先看下现在的问题，假设假设$x_n \in \mathbb{R}^k$

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

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

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

从这点可以想到

$$
\tilde{w} = \begin{bmatrix} w \\ \sqrt{2C}\xi_1 \\ \cdots \\ \sqrt{2C}\xi_N \end{bmatrix}
$$

从而

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

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

$$y_n(w^Tx_n+b)\geq 1-\xi_n \Leftrightarrow$$
$$y_n(w^Tx_n+b+y_n\xi_n)\geq 1 \Leftrightarrow$$
$$y_n(w^Tx_n+\sqrt{2C}\xi_n(\frac{1}{\sqrt{2C}}y_n)+b)\geq 1$$

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

$$\tilde{x}_n=\begin{bmatrix} x_n \\ 0 \\ \cdots \\ \frac{1}{\sqrt{2C}}y_n \\ \cdots \\ 0 \end{bmatrix}\in\mathbb{R}^{k+N}$$

其中$\tilde{x}_n$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

$$\min_{w,b,\xi} \quad \frac{1}{2}\tilde{w}^T\tilde{w}$$
$$\text{subject to} \quad y_n(\tilde{w}^Tx_n+b)\geq 1$$

如果已经计算出了$\tilde{w}$，那么由于

$$\tilde{w}=\begin{bmatrix} w \\ \sqrt{2C}\xi_1 \\ \cdots \\ \sqrt{2C}\xi_N \end{bmatrix}$$

所以取$\tilde{w}$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$M=M_1+M_2$

$$y^TMy=y^T(M_1+M_2)y=y^TM_1y+y^TM_2y\geq 0$$

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

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

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。

$$\begin{aligned}K(x,x^{'})=K_1(x,x^{'})K_2(x,x^{'})&=\phi_1(x)^T\phi_1(x^{'})\phi_2(x)^T\phi_2(x^{'})\\&=\sum_{i=1}^{n}\phi_1^i(x)\phi_1^i(x^{'})\sum_{j=1}^{n}\phi_2^j(x)\phi_2^j(x^{'})\\&=\sum_{i=1}^{n}\sum_{j=1}^{n}\phi_1^i(x)\phi_1^i(x^{'})\phi_2^j(x)\phi_2^j(x^{'})\\&=\sum_{i=1}^{n}\sum_{j=1}^{n}(\phi_1^i(x)\phi_2^j(x))(\phi_1^i(x^{'})\phi_2^j(x^{'}))\end{aligned}$$

根据这个形式，可以做以下定义

$$\Phi^i(x)=\phi_1^i(x)(\phi_2^1(x),\dots,\phi_2^n(x))^T$$
$$\Phi(x)=(\Phi^1(x),\dots,\Phi^n(x))^T$$

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

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

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)

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

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)

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

M的行列式小于0，所以$K(x, x^{'}) = \exp(-K_1(x, x^{'}))$不是kernel

(d)利用$f(x) = \frac{1}{1-x}$在$(0, 1)$区间的泰勒展开可得

$$\begin{aligned} K(x, x^{'}) &= (1 - K_1(x, x^{'}))^{-1} \\ &= \sum_{i=0}^{+\infty} (K_1(x, x^{'}))^i \end{aligned}$$

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

$$\underset{\alpha \in R^N}{\text{minimize}} : \frac{1}{2} \alpha^T Q_D \alpha - 1_N^T \alpha$$

$$\text{subject to} : A_D \alpha \geq u$$

$$Q_D = \begin{bmatrix} y_1 y_1 K_{11} & \dots & y_1 y_N K_{1N} \\ y_2 y_1 K_{12} & \dots & y_2 y_N K_{2N} \\ \dots & \dots & \dots \\ y_N y_1 K_{N1} & \dots & y_N y_N K_{NN} \end{bmatrix}, A_D = \begin{bmatrix} y^T \\ -y^T \\ I_{N \times N} \\ -I_{N \times N} \end{bmatrix}, u = \begin{bmatrix} 0 \\ 0 \\ 0_{N \times N} \\ C \times I_{N \times N} \end{bmatrix}$$

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

$$\begin{aligned} \tilde{Q}_D &= \begin{bmatrix} y_1 y_1 \tilde{K}_{11} & \dots & y_1 y_N \tilde{K}_{1N} \\ y_2 y_1 \tilde{K}_{12} & \dots & y_2 y_N \tilde{K}_{2N} \\ \dots & \dots & \dots \\ y_N y_1 \tilde{K}_{N1} & \dots & y_N y_N \tilde{K}_{NN} \end{bmatrix} \\ &= \begin{bmatrix} y_1 y_1 (pK_{11} + q) & \dots & y_1 y_N (pK_{1N} + q) \\ y_2 y_1 (pK_{12} + q) & \dots & y_2 y_N (pK_{2N} + q) \\ \dots & \dots & \dots \\ y_N y_1 (pK_{N1} + q) & \dots & y_N y_N (pK_{NN} + q) \end{bmatrix} \\ &= pQ_D + q(y_1, \dots, y_N)^T (y_1, \dots, y_N) \end{aligned}$$

$$\tilde{A}_D = A_D$$

$$\tilde{u} = \begin{bmatrix} 0 \\ 0 \\ 0_{N \times N} \\ \tilde{C} \times I_{N \times N} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0_{N \times N} \\ \frac{C}{p} \times I_{N \times N} \end{bmatrix} = \frac{1}{p} u$$

接着我们来计算$\alpha^T \tilde{Q}_D \alpha$

$$\text{注意}(y_1,\dots,y_N)\alpha=0$$
$$\text{所以}\alpha^T\tilde{Q}_D\alpha=\alpha^TpQ_D\alpha+\alpha^Tq(y_1,\dots,y_N)^T(y_1,\dots,y_N)\alpha=p\alpha^TQ_D\alpha$$

所以我们的目标函数为

$$\frac{1}{2}\alpha^T\tilde{Q}_D\alpha-1_N^T\alpha=\frac{1}{2}p\alpha^T\tilde{Q}_D\alpha-1_N^T\alpha=\frac{1}{p}[\frac{1}{2}(p\alpha)^TQ_D(p\alpha)-1_N^T(p\alpha)]$$

由于p为常数，所以目标函数可以简化为

$$\frac{1}{2}(p\alpha)^TQ_D(p\alpha)-1_N^T(p\alpha)$$

再看下限制条件

$$\tilde{A}_D\alpha\geq\tilde{u}\Leftrightarrow A_D\alpha\geq\frac{1}{p}u\Leftrightarrow A_D(p\alpha)\geq u$$

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

$$\underset{\alpha\in R^N}{\text{minimize}}:\frac{1}{2}\overline{\alpha}^TQ_D\overline{\alpha}-1_N^T\overline{\alpha}$$
$$\text{subject to}:A_D\overline{\alpha}\geq u$$
$$Q_D=\begin{bmatrix}y_1y_1K_{11}&\dots&y_1y_NK_{1N}\\y_2y_1K_{12}&\dots&y_2y_NK_{2N}\\\dots&\dots&\dots\\y_Ny_1K_{N1}&\dots&y_Ny_NK_{NN}\end{bmatrix},A_D=\begin{bmatrix}y^T\\-y^T\\I_{N\times N}\\-I_{N\times N}\end{bmatrix},u=\begin{bmatrix}0\\0\\0_{N\times N}\\C\times I_{N\times N}\end{bmatrix}$$

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α^*，那么该问题的最优解$\tilde{\alpha}^*$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

$$w^*=\sum_{n=1}^{N}\alpha_n^*y_nz_n$$
$$\beta_n^*=C-\alpha_n^*(n=1,\dots,N)$$
$$b^*=y_m-w^{*T}z_m=y_m-(\sum_{n=1}^{N}\alpha_n^*y_nz_n)^Tz_m=y_m-\sum_{n=1}^{N}\alpha_n^*y_nK(x_n,x_m)$$
$$\text{其中}z_m\text{对应的}\alpha_m^*\neq0$$
$$g(x)=\text{sign}(w^{*T}z+b)=\text{sign}((\sum_{n=1}^{N}\alpha_n^*y_nz_n)^Tz+b)=\text{sign}(\sum_{n=1}^{N}\alpha_n^*y_nK(x_n,x)+b^*)$$

如果我们将kernel换成

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

利用之前的条件$\alpha^*=p\tilde{\alpha}^*$以及$\tilde{C}=\frac{C}{p},\sum_{n=1}^{N}\alpha_n^*y_n=0$，可以对变换kernel之后的问题求解

$$\tilde{w}^* = \sum_{n=1}^{N} \tilde{\alpha}_n^* y_n z_n = \frac{1}{p}(\sum_{n=1}^{N} \alpha_n^* y_n z_n) = \frac{w^*}{p}$$

$$\tilde{\beta}_n^* = \tilde{C} - \tilde{\alpha}_n^* = \frac{C}{p} - \frac{\alpha_n^*}{p} = \frac{1}{p}(C - \alpha_n^*) = \frac{\beta_n}{p}(n = 1, \ldots, N)$$

$$\begin{aligned}
\tilde{b}^* &= y_m - \sum_{n=1}^{N} \tilde{\alpha}_n^* y_n \tilde{K}(x_n, x_m) \\
&= y_m - \sum_{n=1}^{N} \frac{\alpha_n^*}{p} y_n (pK(x_n, x_m) + q) \\
&= y_m - \sum_{n=1}^{N} \alpha_n^* y_n K(x_n, x_m) - \frac{q}{p} \sum_{n=1}^{N} \alpha_n^* y_n \\
&= y_m - \sum_{n=1}^{N} \alpha_n^* y_n K(x_n, x_m) \\
&= b^*
\end{aligned}$$

$$\begin{aligned}
\tilde{g}(x) &= \text{sign}(\sum_{n=1}^{N} \tilde{\alpha}_n^* y_n \tilde{K}(x_n, x) + \tilde{b}^*) \\
&= \text{sign}[\sum_{n=1}^{N} \frac{\alpha_n^*}{p} y_n (pK(x_n, x) + q) + b^*] \\
&= \text{sign}[\sum_{n=1}^{N} \alpha_n^* y_n K(x_n, x) + \frac{q}{p} \sum_{n=1}^{N} \alpha_n^* y_n + b^*] \\
&= \text{sign}(\sum_{n=1}^{N} \alpha_n^* y_n K(x_n, x) + b^*) \\
&= g(x)
\end{aligned}$$

这说明这样变换之后我们的分类器没有变。

Problem 15

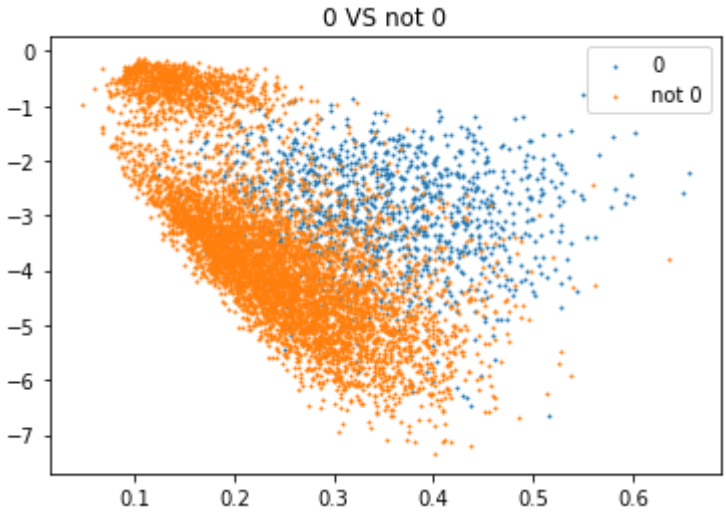
首先读取数据

```
import matplotlib.pyplot as plt
import numpy as np

def transformdata(file):
    X = []
    Y = []
    with open(file) as data:
        for i in data.readlines():
            j = list(map(float,i.strip().split()))
            y = j[0]
            x = j[1:]
            Y.append(y)
            X.append(x)
    return np.array(X),np.array(Y)
```

```
train = "featurestrain.txt"
X_train,Y_trian = transformdata(train)
test = "featurestest.txt"
X_test,Y_test = transformdata(test)
```

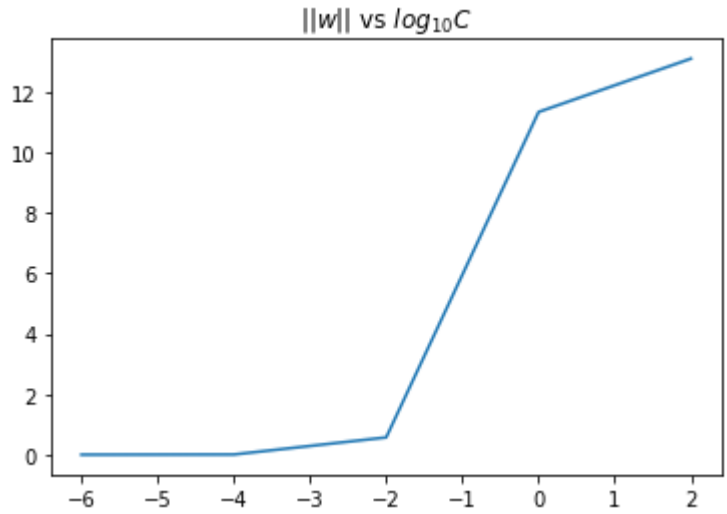
注意此题是区分0和非0，作图看下。

```
x1 = X_train[Y_trian==0][:,0]
y1 = X_train[Y_trian==0][:,1]
x2 = X_train[Y_trian!=0][:,0]
y2 = X_train[Y_trian!=0][:,1]

plt.scatter(x1,y1,s=1,label = '0')
plt.scatter(x2,y2,s=1,label = 'not 0')
plt.title('0 VS not 0')
plt.legend()
plt.show()
```



现在可以训练模型并作图了。

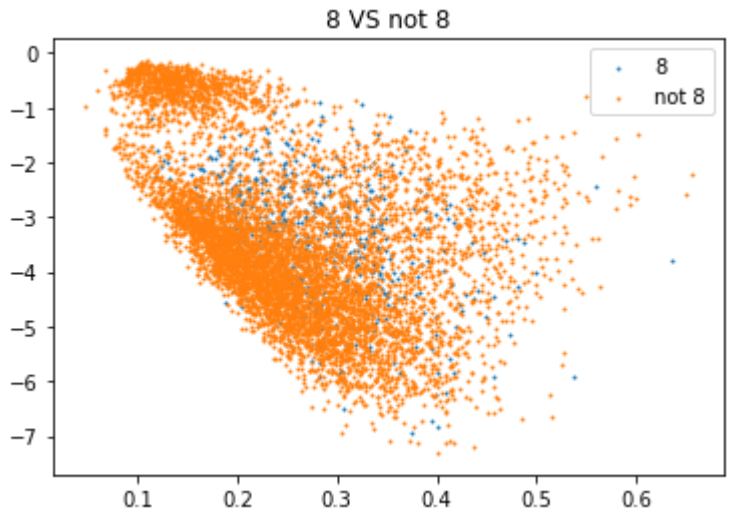
```
Y_trian1 = (Y_trian==0)
C = [-6,-4,-2,0,2]
W = []

for i in C:
    c = 10**i
    clf = svm.SVC(kernel = "linear",C = c)
    clf.fit(X_train,Y_trian1)
    w = clf.coef_[0]
    W = np.append(W,np.sqrt(np.sum(w*w)))

plt.plot(C,W)
plt.title("$||w||$ vs $log_{10}C$")
plt.show()
```



Problem 16

注意这题是8和not 8

```
x3 = X_train[Y_trian==8][:,0]
y3 = X_train[Y_trian==8][:,1]

x4 = X_train[Y_trian!=8][:,0]
y4 = X_train[Y_trian!=8][:,1]

plt.scatter(x3,y3,s=1,label = '8')
plt.scatter(x4,y4,s=1,label = 'not 8')
plt.title('8 VS not 8')
plt.legend()
plt.show()
```

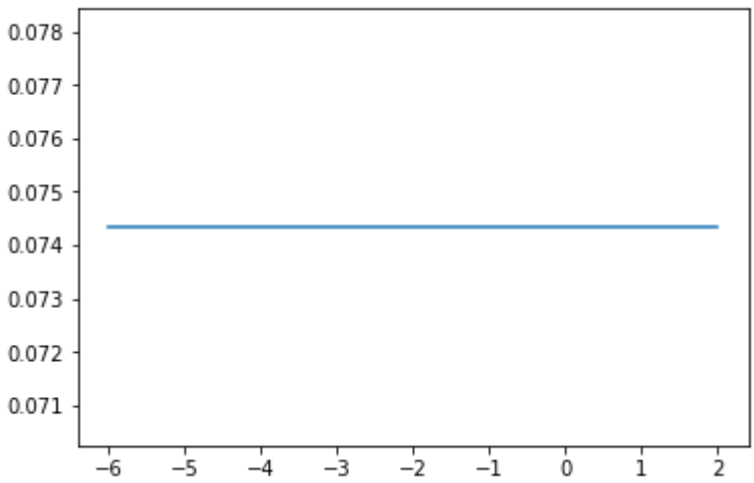


注意17题要计算$\sum_{n=1}^{N}\alpha_n$，所以我们这题把系数也算出来， 由于sklearn只能计算对偶系数$y_n\alpha_n$，所以这里要把标签转换为$+1,-1$，方便计算。

```
Y_trian2 = 2*(Y_trian==8)-1

C = [-6,-4,-2,0,2]
Ein = []
alpha = []

for i in C:
    c = 10**i
    clf = svm.SVC(kernel='poly',degree=2,coef0=1,gamma=1,C = c)
    clf.fit(X_train,Y_trian2)
    e = np.sum(clf.predict(X_train) != Y_trian2)/len(X_train)
    support = clf.support_
    coef = np.sum(clf.dual_coef_[0]*Y_trian2[support])
    alpha.append(coef)
    Ein.append(e)
```

作图。

```
plt.plot(C,Ein)
plt.show()
```

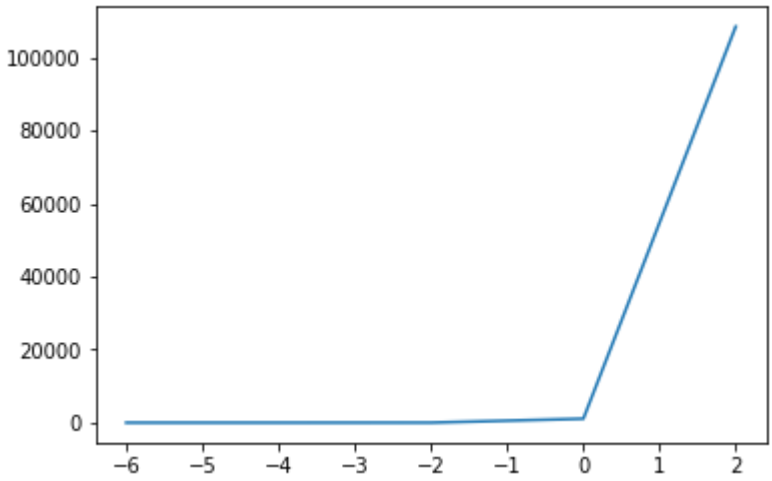


比较奇特的是这题的E_{in}都一样。

Problem 17

利用上题的数据作图即可。

```
plt.plot(C,alpha)
plt.show()
```

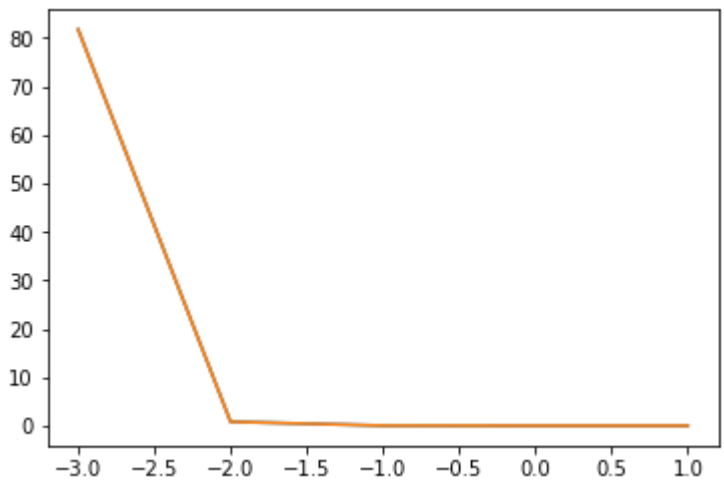


可以看到尽管上题的E_{in}一致，但是这里$\sum_{n=1}^{N} \alpha_n$会增加。

Problem 18

这题要计算距离，注意距离为$\frac{1}{||w||}$

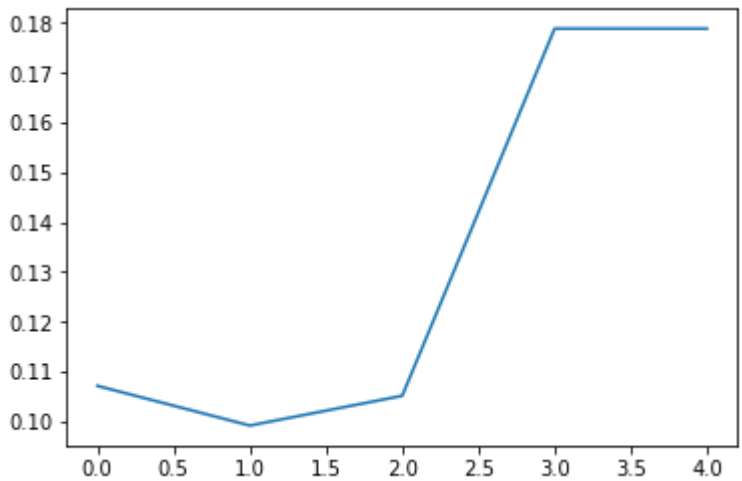
```
C = [-3,-2,-1,0,1]
Distance = []

for i in C:
    c = 10**i
    clf = svm.SVC(kernel='rbf',gamma=1,C = c)
    clf.fit(X_train,Y_trian1)
    w = clf.dual_coef_[0].dot(clf.support_vectors_)
    distance = 1/np.sum(w*w)
    Distance.append(distance)

plt.plot(C, Distance)
plt.show()
```



随着γ增加，距离超平面的距离在减少。

Problem 19

```
Y_test1 = (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_trian1)
    e = np.sum(clf.predict(X_test) != Y_test1)/len(X_test)
    Eout.append(e)

plt.plot(Gamma,Eout)
plt.show()
```



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

Problem 20

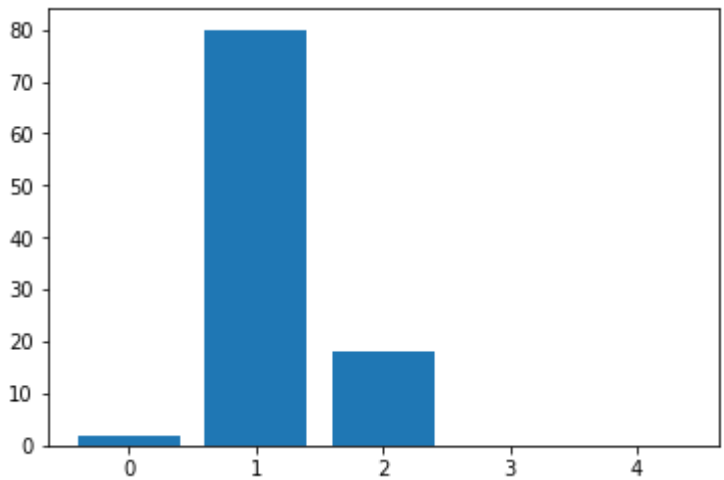
这题要构造交叉验证集，多次实验，做直方图，先做一些预处理。

```
from sklearn.model_selection import train_test_split

#对数据合并，方便调用train_test_split函数
Data = np.concatenate((X_train,Y_trian1.reshape(-1,1)),axis=1)
N = 100
Cnt = np.zeros(5)
Gamma = range(5)

for _ in range(N):
    train_set, val_set = train_test_split(Data, test_size=0.2)
    #取特征
```

```
    Xtrain = train_set[:,:2]
    #取标签
    Ytrain = train_set[:,2]
    Xval = val_set[:,:2]
    Yval = val_set[:,2]
    Eval = np.array([])

    for i in Gamma:
        gamma = 10**i
        clf = svm.SVC(kernel='rbf',gamma=gamma,C = 0.1)
        clf.fit(Xtrain,Ytrain)
        e = np.sum(clf.predict(Xval) != Yval)/len(Xval)
        Eval = np.append(Eval,e)
    index = np.argmin(Eval)
    Cnt[index] += 1
```

作图

```
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对偶问题的的对偶问题，我们来看一下。

首先回顾下hard-margin SVM对偶问题。

$$\underset{\alpha\in R^N}{\text{minimize}}:\frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}y_n y_m \alpha_n \alpha_m x_n^T x_m-\sum_{n=1}^{N}\alpha_n$$

$$\text{subject to}:\sum_{n=1}^{N}y_n\alpha_n=0,\alpha_n\geq 0(n=1,\dots,N)$$

根据拉格朗日乘子法，我们将上述问题转化为

$$\min_{\alpha\in R^N}\max_{\lambda_i\geq 0}:\frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}y_ny_m\alpha_n\alpha_mx_n^Tx_m-\sum_{n=1}^{N}\alpha_n+\lambda_0(\sum_{n=1}^{N}y_n\alpha_n)-\sum_{n=1}^{N}\lambda_n\alpha_n$$

这里肯定是默认KKT条件成立，所以上述问题可以转化为

$$\max_{\lambda_i\geq 0}\min_{\alpha\in R^N}:\frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}y_ny_m\alpha_n\alpha_mx_n^Tx_m-\sum_{n=1}^{N}\alpha_n+\lambda_0(\sum_{n=1}^{N}y_n\alpha_n)-\sum_{n=1}^{N}\lambda_n\alpha_n$$

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

$$f(\lambda,\alpha)=\frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}y_ny_m\alpha_n\alpha_mx_n^Tx_m-\sum_{n=1}^{N}\alpha_n+\lambda_0(\sum_{n=1}^{N}y_n\alpha_n)-\sum_{n=1}^{N}\lambda_n\alpha_n$$

关于α_i求偏导可得

$$\begin{aligned}\frac{\partial f}{\partial\alpha_i}&=\frac{1}{2}\sum_{n=1}^{N}y_ny_i\alpha_nx_n^Tx_i+\frac{1}{2}\sum_{m=1}^{N}y_iy_m\alpha_mx_i^Tx_m-1+\lambda_0y_i-\lambda_i\\&=\sum_{n=1}^{N}y_ny_i\alpha_nx_i^Tx_n-1+\lambda_0y_i-\lambda_i\end{aligned}$$

令偏导为0可得

$$\sum_{n=1}^{N}y_ny_i\alpha_nx_i^Tx_n=1-\lambda_0y_i+\lambda_i$$

对这个式子作以下变形可得

$$\begin{bmatrix}y_iy_1x_i^Tx_1&\dots&y_iy_Nx_i^Tx_N\end{bmatrix}\begin{bmatrix}\alpha_1\\\dots\\\alpha_N\end{bmatrix}=1-\lambda_0y_i+\lambda_i\tag{1}$$

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

$$\begin{gathered}\underset{\alpha\in R^N}{\text{minimize}}:\frac{1}{2}\alpha^TQ_D\alpha-1_N^T\alpha\\\text{subject to}:A_D\alpha\geq 0_{N+2}\\Q_D=\begin{bmatrix}y_1y_1x_1^Tx_1&\dots&y_1y_Nx_1^Tx_N\\y_2y_1x_2^Tx_1&\dots&y_2y_Nx_2^Tx_N\\\dots&\dots&\dots\\y_Ny_1x_N^Tx_1&\dots&y_Ny_Nx_N^Tx_N\end{bmatrix}\text{ and }A_D=\begin{bmatrix}y^T\\-y^T\\I_{N\times N}\end{bmatrix}\end{gathered}$$

(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

$$\begin{gathered}Q_D\alpha=1_N-\lambda_0y+\lambda\\\alpha=\begin{bmatrix}\alpha_1\\\dots\\\alpha_N\end{bmatrix},y=\begin{bmatrix}y_1\\\dots\\y_N\end{bmatrix},\lambda=\begin{bmatrix}\lambda_1\\\dots\\\lambda_N\end{bmatrix}\end{gathered}$$

在这个记号下，我们问题改写下

$$f(\lambda,\alpha)=\frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}y_ny_m\alpha_n\alpha_mx_n^Tx_m-\sum_{n=1}^{N}\alpha_n+\lambda_0(\sum_{n=1}^{N}y_n\alpha_n)-\sum_{n=1}^{N}\lambda_n\alpha_n$$

$$\sum_{m=1}^{N}\sum_{n=1}^{N}y_ny_m\alpha_n\alpha_mx_n^Tx_m=\alpha^TQ_D\alpha$$

$$1_N^T\alpha=\sum_{n=1}^{N}\alpha_n$$

$$\lambda_0(\sum_{n=1}^{N}y_n\alpha_n)=\lambda_0\alpha^Ty$$

$$\sum_{n=1}^{N}\lambda_n\alpha_n=\alpha^T\lambda$$

$$f(\lambda,\alpha)=\frac{1}{2}\alpha^TQ_D\alpha-1_N^T\alpha+\lambda_0\alpha^Ty-\alpha^T\lambda$$

将$Q_D\alpha=1_N-\lambda_0y+\lambda$带入可得

$$\begin{aligned}f(\lambda,\alpha)&=\frac{1}{2}\alpha^TQ_D\alpha-1_N^T\alpha+\lambda_0\alpha^Ty-\alpha^T\lambda\\&=\frac{1}{2}\alpha^T(1_N-\lambda_0y+\lambda)-1_N^T\alpha+\lambda_0\alpha^Ty-\alpha^T\lambda\\&=-\frac{1}{2}\alpha^T1_N+\frac{1}{2}\lambda_0\alpha^Ty-\frac{1}{2}\alpha^T\lambda\\&=-\frac{1}{2}\alpha^T(1_N-\lambda_0y+\lambda)\end{aligned}$$

如果Q_D可逆，那么

$$\alpha=Q_D^{-1}(1_N-\lambda_0y+\lambda)$$

代入可得

$$\begin{aligned}-\frac{1}{2}\alpha^T(1_N-\lambda_0y+\lambda)&=-\frac{1}{2}[Q_D^{-1}(1_N-\lambda_0y+\lambda)]^T(1_N-\lambda_0y+\lambda)\\&=-\frac{1}{2}(1_N-\lambda_0y+\lambda)^TQ_D^{-1}(1_N-\lambda_0y+\lambda)\end{aligned}$$

所以问题转化为

$$\begin{aligned}\underset{\lambda_i\geq0}{\text{maxmize}}:&-\frac{1}{2}(1_N-\lambda_0y+\lambda)^TQ_D^{-1}(1_N-\lambda_0y+\lambda)\\\text{subject to}:&\lambda_i\geq0(n=0,1,\dots,N)\end{aligned}$$

把负号提出来，可以转化为标准的QP问题

$$\begin{aligned}\underset{\lambda_i\geq0}{\text{minmize}}:&\frac{1}{2}(1_N-\lambda_0y+\lambda)^TQ_D^{-1}(1_N-\lambda_0y+\lambda)\\\text{subject to}:&\lambda_i\geq0(n=0,1,\dots,N)\end{aligned}$$

可以看到，这和最开始的问题是非常类似的。