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

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

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

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

一共$d + N + 1$个。限制条件为

$$
\begin{aligned}
y_n (w^T x_n + b) \ge 1 - \xi_n \\
\xi_n \ge 0 (n = 1, \ldots, N)
\end{aligned}
$$

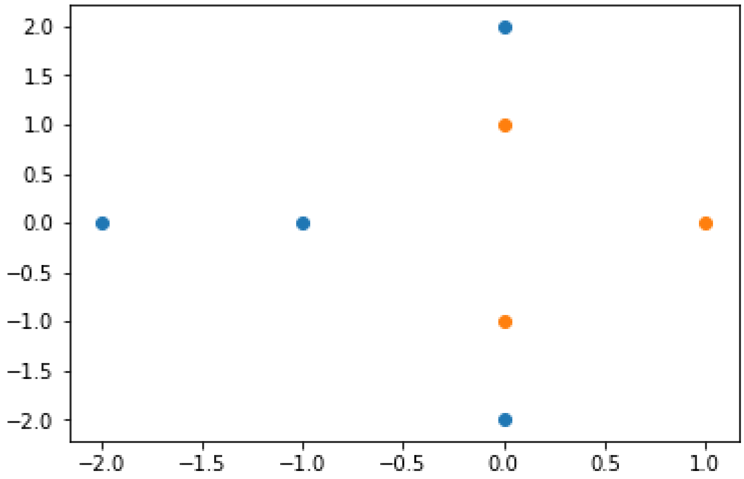
一共有$2N$个。

Problem 2

首先作图看下

```python
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

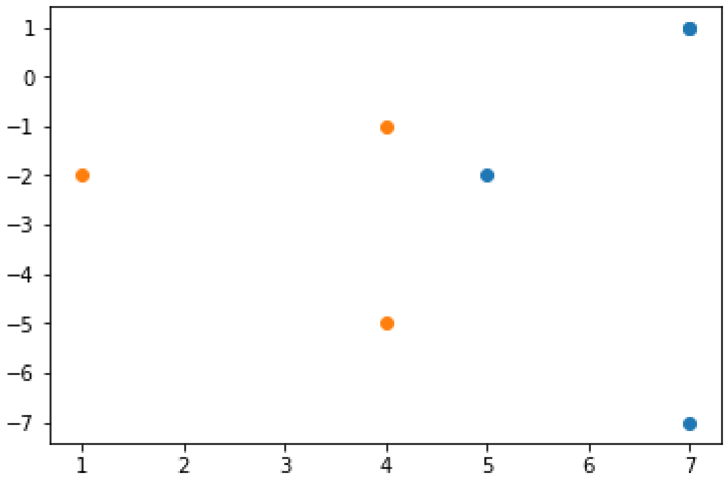
$$z_4 = (5,-2), z_5 = (7,-7), z_6 = (7,1), z_7 = (7,1)$$

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()
```

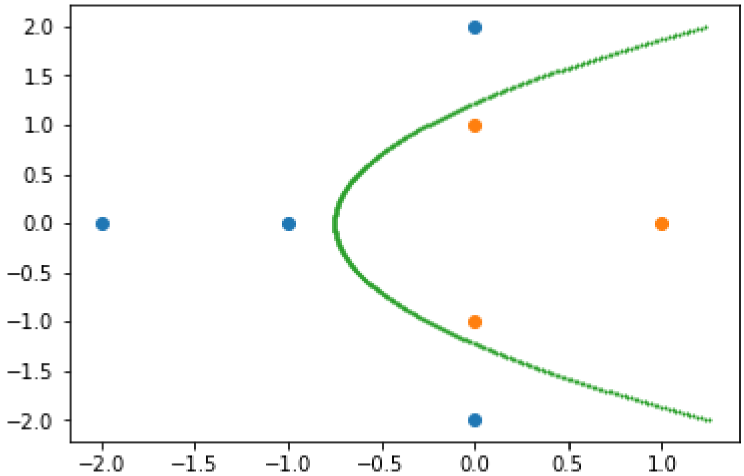


从这个图像中可以看出，最大间隔分类器为$\varphi_1(x) = 4.5$，将$\varphi_1(x) = x_2^2 - 2x_1 + 3$带入可得最大间隔分类器为

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

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

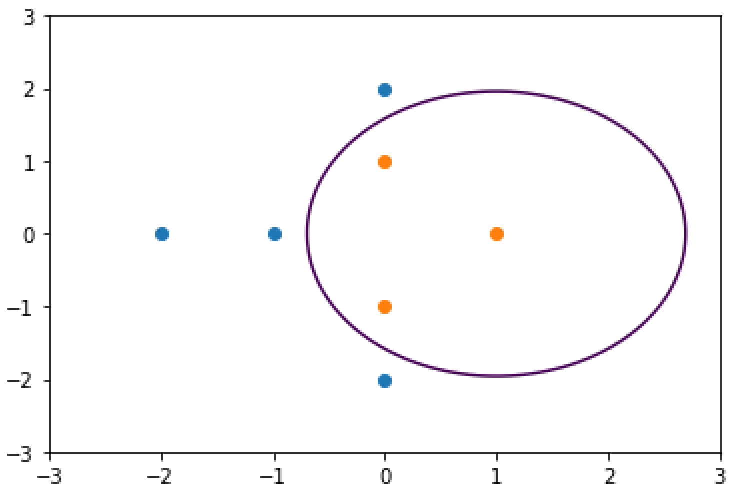
$$k^T z + b = 0$$

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

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

所以在$||x_n-c||^2\le R^2$条件下

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

从而

$$\min_{R\in\mathbb{R},c\in\mathbb{R}^d}\ \max_{\lambda_n\ge0} L(R,c,\lambda)=\min_{R\in\mathbb{R},c\in\mathbb{R}^d} R^2$$

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

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

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

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

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

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

再带入$c=\sum_{n=1}^{N}\lambda_n x_n$

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

所以问题转换为

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

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

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

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，

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

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

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

所以如果存在$\lambda_i \neq 0$，那么

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

结合$c = \sum_{n=1}^{N} \lambda_n z_n$，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

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

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

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

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

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

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

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

如果已经计算出了$\tilde w$，那么由于

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

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$M=M_1+M_2$

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

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

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

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kernele

(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

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

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

$$
\begin{aligned}
\tilde{Q}_D&=\begin{bmatrix}y_1y_1\tilde{K}_{11} & \ldots & y_1y_N\tilde{K}_{1N}\\y_2y_1\tilde{K}_{12} & \ldots & y_2y_N\tilde{K}_{2N}\\\ldots & \ldots & \ldots\\y_Ny_1\tilde{K}_{N1} & \ldots & y_Ny_N\tilde{K}_{NN}\end{bmatrix}\\
&=\begin{bmatrix}y_1y_1(pK_{11}+q) & \ldots & y_1y_N(pK_{1N}+q)\\y_2y_1(pK_{12}+q) & \ldots & y_2y_N(pK_{2N}+q)\\\ldots & \ldots & \ldots\\y_Ny_1(pK_{N1}+q) & \ldots & y_Ny_N(pK_{NN}+q)\end{bmatrix}\\
&=pQ_D+q(y_1,\ldots,y_N)^T(y_1,\ldots,y_N)\\
\tilde{A}_D&=A_D\\
\tilde{u}&=\begin{bmatrix}0\\0\\0_{N\times N}\\\tilde{C}\times I_{N\times N}\end{bmatrix}=\begin{bmatrix}0\\0\\0_{N\times N}\\\frac{C}{p}\times I_{N\times N}\end{bmatrix}=\frac{1}{p}u
\end{aligned}
$$

接着我们来计算$\alpha^T\tilde{Q}_D\alpha$

$$\text{注意}(y_1,\ldots,y_N)\alpha = 0$$
$$\text{所以}\,\alpha^T\tilde{Q}_D\alpha = \alpha^T pQ_D\alpha + \alpha^T q(y_1,\ldots,y_N)^T(y_1,\ldots,y_N)\alpha = p\alpha^T Q_D\alpha$$

所以我们的目标函数为

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

由于p为常数，所以目标函数可以简化为

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

再看下限制条件

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

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

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

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

$$w^* = \sum_{n=1}^N \alpha_n^* y_n z_n$$
$$\beta_n^* = C - \alpha_n^*(n = 1,\ldots,N)$$
$$b^* = y_m - w^{*T}z_m = y_m - (\sum_{n=1}^N \alpha_n^* y_n z_n)^T z_m = y_m - \sum_{n=1}^N \alpha_n^* y_n K(x_n, x_m)$$
$$\text{其中}\,z_m\text{对应的}\,\alpha_m^* \ne 0$$
$$g(x) = \text{sign}(w^{*T}z + b) = \text{sign}((\sum_{n=1}^N \alpha_n^* y_n z_n)^T z + b) = \text{sign}(\sum_{n=1}^N \alpha_n^* y_n K(x_n, x) + b^*)$$

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

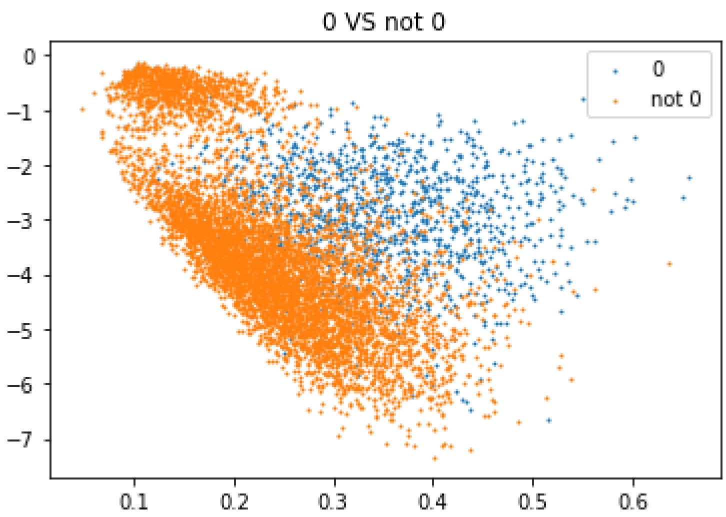
首先读取数据

```
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)
```

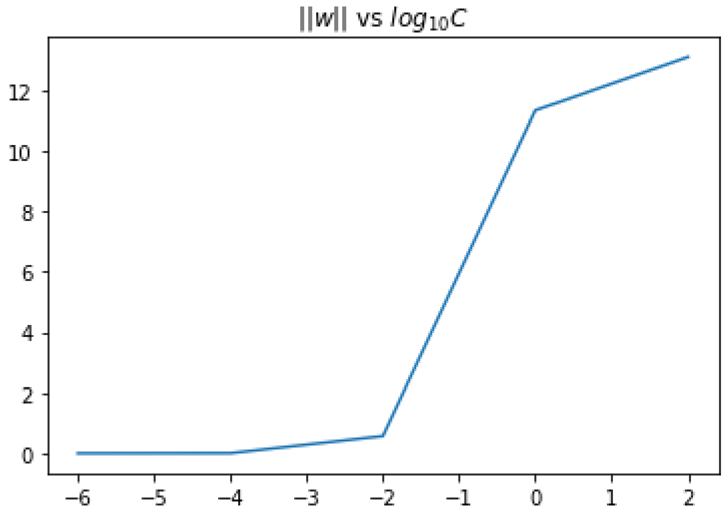
注意此题是区分0和非0，作图看下。

```
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。

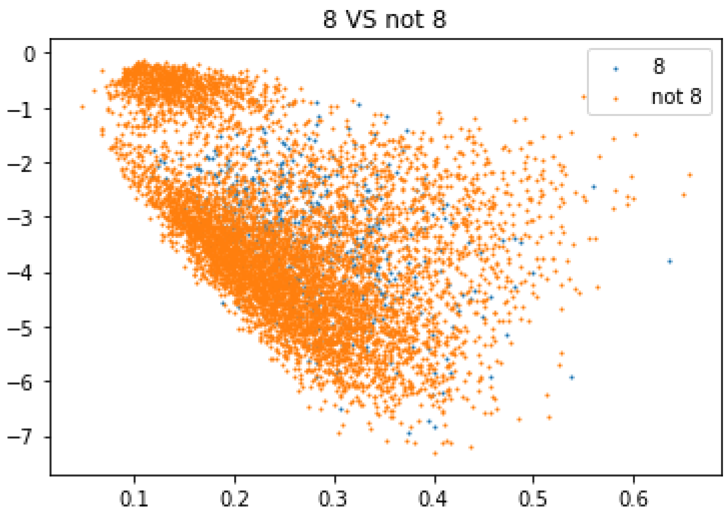
```
Y_trian1 = (Y_trian==0)
C = [-6,-4,-2,0,2]
W = []

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()
```

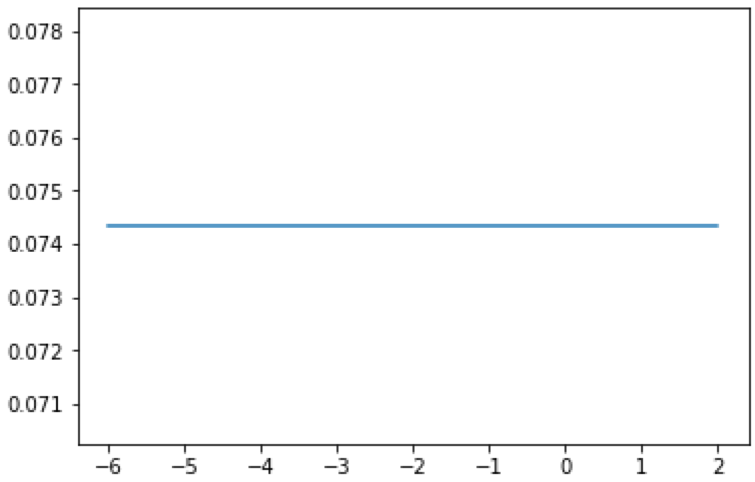


注意17题要计算$\sum_{n=1}^{N}\alpha_n$，所以我们这题把系数也算出来， 由于sklearn只能计算对偶系数$y_n\alpha_n$，所以这里要把标签转换为$+1,-1$，方便计算。

```
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()
```

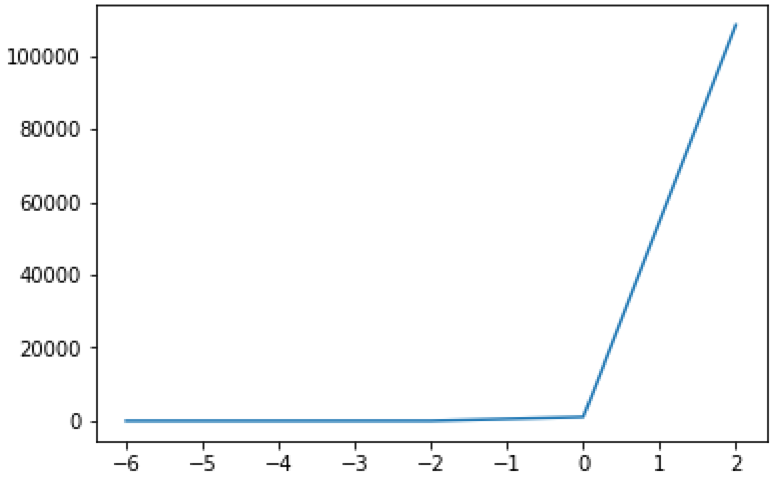


比较奇特的是这题的E_{in}都一样。

Problem 17

利用上题的数据作图即可。

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

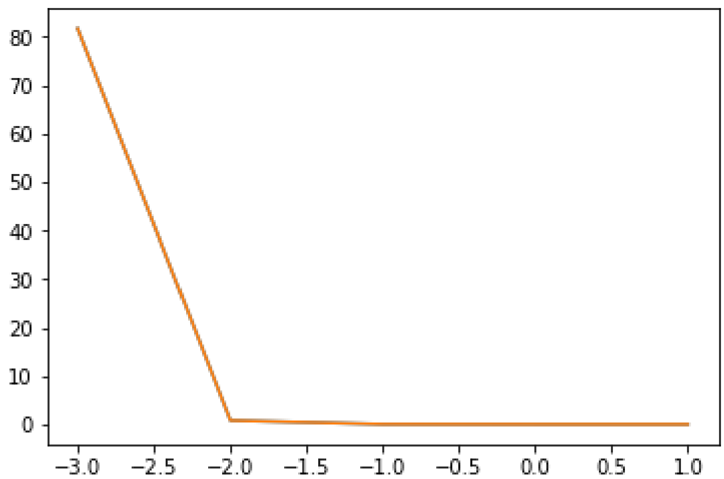


可以看到尽管上题的E_{in}一致，但是这里$\sum_{n=1}^{N}\alpha_n$会增加。

Problem 18

这题要计算距离，注意距离为$\frac{1}{||w||}$

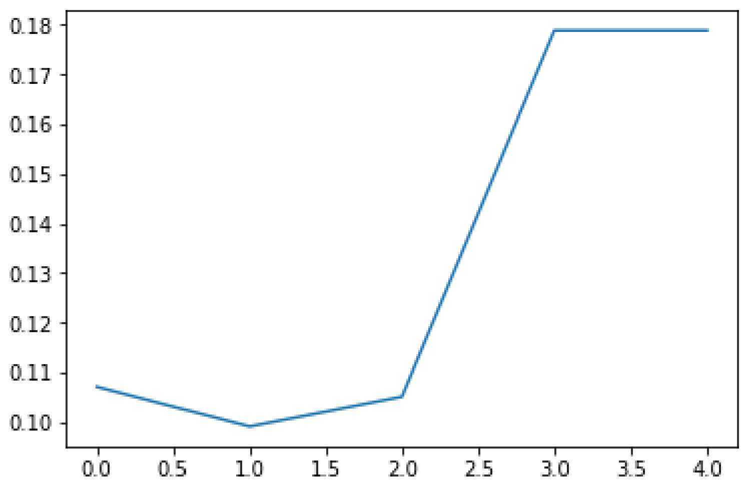
```
C = [-3,-2,-1,0,1]
Distance = []

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

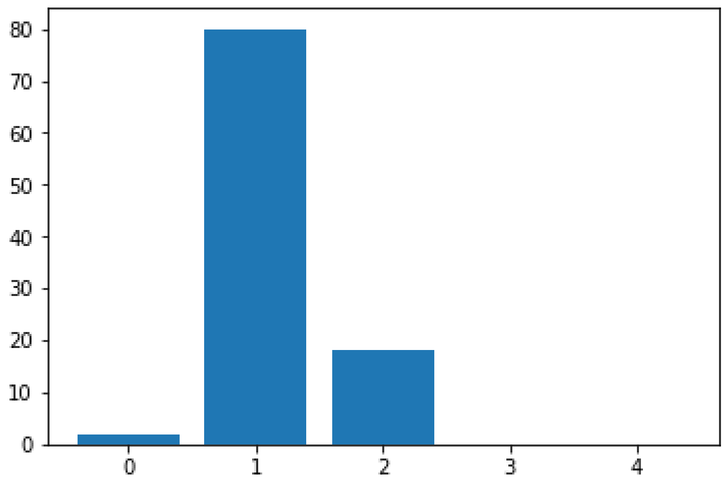
这题要构造交叉验证集，多次实验，做直方图，先做一些预处理。

```
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。

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

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

根据拉格朗日乘子法，我们将上述问题转化为

$$\min_{\alpha\in R^N}\max_{\lambda_i\ge 0}:\frac{1}{2}\sum_{m=1}^N\sum_{n=1}^N y_n y_m\alpha_n\alpha_m x_n^T x_m-\sum_{n=1}^N\alpha_n+\lambda_0(\sum_{n=1}^N y_n\alpha_n)-\sum_{n=1}^N\lambda_n\alpha_n$$

这里肯定是默认KKT条件成立，所以上述问题可以转化为

$$\max_{\lambda_i\ge 0}\min_{\alpha\in R^N}:\frac{1}{2}\sum_{m=1}^N\sum_{n=1}^N y_n y_m\alpha_n\alpha_m x_n^T x_m-\sum_{n=1}^N\alpha_n+\lambda_0(\sum_{n=1}^N y_n\alpha_n)-\sum_{n=1}^N\lambda_n\alpha_n$$

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

$$f(\lambda,\alpha)=\frac{1}{2}\sum_{m=1}^N\sum_{n=1}^N y_n y_m\alpha_n\alpha_m x_n^T x_m-\sum_{n=1}^N\alpha_n+\lambda_0(\sum_{n=1}^N y_n\alpha_n)-\sum_{n=1}^N\lambda_n\alpha_n$$

关于α_i求偏导可得

$$\begin{aligned}\frac{\partial f}{\partial\alpha_i}&=\frac{1}{2}\sum_{n=1}^N y_n y_i\alpha_n x_n^T x_i+\frac{1}{2}\sum_{m=1}^N y_i y_m\alpha_m x_i^T x_m-1+\lambda_0 y_i-\lambda_i\\&=\sum_{n=1}^N y_n y_i\alpha_n x_i^T x_n-1+\lambda_0 y_i-\lambda_i\end{aligned}$$

令偏导为0可得

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

对这个式子作以下变形可得

$$\begin{bmatrix} y_i y_1 x_i^T x_1 & \ldots & y_i y_N x_i^T x_N\end{bmatrix}\begin{bmatrix}\alpha_1\\ \ldots\\ \alpha_N\end{bmatrix}=1-\lambda_0 y_i+\lambda_i \tag{1}$$

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

$$\begin{gathered}\underset{\alpha\in R^N}{\text{minimize}}:\frac{1}{2}\alpha^T Q_D\alpha-1_N^T\alpha\\ \text{subject to}:A_D\alpha\ge 0_{N+2}\\ Q_D=\begin{bmatrix} y_1 y_1 x_1^T x_1 & \ldots & y_1 y_N x_1^T x_N\\ y_2 y_1 x_2^T x_1 & \ldots & y_2 y_N x_2^T x_N\\ \ldots & \ldots & \ldots\\ y_N y_1 x_N^T x_1 & \ldots & y_N y_N x_N^T x_N\end{bmatrix}\text{ and }A_D=\begin{bmatrix} y^T\\ -y^T\\ I_{N\times N}\end{bmatrix}\end{gathered}$$

(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

$$\begin{gathered}Q_D\alpha=1_N-\lambda_0 y+\lambda\\ \alpha=\begin{bmatrix}\alpha_1\\ \ldots\\ \alpha_N\end{bmatrix},y=\begin{bmatrix}y_1\\ \ldots\\ y_N\end{bmatrix},\lambda=\begin{bmatrix}\lambda_1\\ \ldots\\ \lambda_N\end{bmatrix}\end{gathered}$$

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

$$\begin{gathered}\underset{\lambda_i\ge0}{\text{maxmize}}:-\frac{1}{2}(1_N-\lambda_0y+\lambda)^TQ_D^{-1}(1_N-\lambda_0y+\lambda)\\\text{subject to}:\lambda_i\ge0(n=0,1,\ldots,N)\end{gathered}$$

把负号提出来，可以转化为标准的QP问题

$$\begin{gathered}\underset{\lambda_i\ge0}{\text{minmize}}:\frac{1}{2}(1_N-\lambda_0y+\lambda)^TQ_D^{-1}(1_N-\lambda_0y+\lambda)\\\text{subject to}:\lambda_i\ge0(n=0,1,\ldots,N)\end{gathered}$$

可以看到，这和最开始的问题是非常类似的。