1.Logistic regression

(a)首先回顾$J(\theta)$的定义

$$J(\theta)=-\frac{1}{m}\sum_{i=1}^{m}\log(h_\theta(y^{(i)}x^{(i)}))$$

$$y(i)\in\{-1,1\},h_\theta(x)=g(\theta^Tx),g(z)=1/(1+e^{-z})$$

注意$g^{'}(z)=g(z)(1-g(z))$，利用这点来求$\frac{\partial h_\theta(x)}{\partial \theta_k}$

$$\begin{aligned}\frac{\partial h_\theta(x)}{\partial \theta_k}&=\frac{\partial g(\theta^Tx)}{\partial \theta_k}\\&=g(\theta^Tx)(1-g(\theta^Tx))\frac{\partial(\theta^Tx)}{\partial \theta_k}\\&=g(\theta^Tx)(1-g(\theta^Tx))x_k\\&=h_\theta(x)(1-h_\theta(x))x_k\end{aligned}$$

利用$\frac{\partial h_\theta(x)}{\partial \theta_k}$来求$\frac{\partial J(\theta)}{\partial \theta_k}$

$$\begin{aligned}\frac{\partial J(\theta)}{\partial \theta_k}&=-\frac{1}{m}\sum_{i=1}^{m}\frac{\partial\log(h_\theta(y^{(i)}x^{(i)}))}{\partial \theta_k}\\&=-\frac{1}{m}\sum_{i=1}^{m}\frac{1}{h_\theta(y^{(i)}x^{(i)}))}\frac{\partial h_\theta(y^{(i)}x^{(i)}))}{\partial \theta_k}\\&=-\frac{1}{m}\sum_{i=1}^{m}\frac{1}{h_\theta(y^{(i)}x^{(i)}))}h_\theta(y^{(i)}x^{(i)})(1-h_\theta(y^{(i)}x^{(i)}))y^{(i)}x_k^{(i)}\\&=-\frac{1}{m}\sum_{i=1}^{m}(1-h_\theta(y^{(i)}x^{(i)}))y^{(i)}x_k^{(i)}\end{aligned}$$

这个形式方便我们求二阶偏导，继续利用$\frac{\partial h_\theta(x)}{\partial \theta_k}$来求$\frac{\partial^2 J(\theta)}{\partial \theta_l\partial \theta_k}$

$$\begin{aligned}\frac{\partial^2 J(\theta)}{\partial \theta_l\partial \theta_k}&=-\frac{1}{m}\sum_{i=1}^{m}y^{(i)}x_k^{(i)}\frac{\partial(1-h_\theta(y^{(i)}x^{(i)}))}{\partial \theta_l}\\&=\frac{1}{m}\sum_{i=1}^{m}y^{(i)}x_k^{(i)}\frac{\partial(h_\theta(y^{(i)}x^{(i)}))}{\partial \theta_l}\\&=\frac{1}{m}\sum_{i=1}^{m}x_k^{(i)}h_\theta(y^{(i)}x^{(i)})(1-h_\theta(y^{(i)}x^{(i)}))x_l^{(i)}\end{aligned}$$

接着作以下记号

$$x_k=[x_1^{(k)},\ldots,x_n^{(k)}]^T\in R^n$$

$$X=\begin{bmatrix}x_1^T\\ \ldots\\ x_m^T\end{bmatrix}\in R^{m\times n}$$

$$\Lambda=\mathrm{diag}\{h_\theta(y^{(1}x^{(1)})(1-h_\theta(y^{(1)}x^{(1)}),\ldots,h_\theta(y^{(m)}x^{(m)})(1-h_\theta(y^{(m)}x^{(m)})\}\in R^{m\times m}$$

所以Hessian矩阵H可以表达为如下形式

$$H = X^T \Lambda X$$

为了(b)题需要，这里也将$\nabla J(\theta)$表示出来

$$S = \begin{bmatrix} (1 - h_\theta(y^{(1)}x^{(1)}))y^{(1)} \\ \ldots \\ (1 - h_\theta(y^{(m)}x^{(m)}))y^{(m)} \end{bmatrix} \in R^m$$

$$\nabla J(\theta) = -\frac{1}{m} X^T S$$

现在任取$z \in R^n$，记$t = X^T z$，那么

$$z^T H z = z^T X \Lambda X^T z = t^T \Lambda t = \sum_{i=1}^m t_i^2 h_\theta(y^{(i)}x^{(i)})(1 - h_\theta(y^{(i)}x^{(i)})$$

注意$h_\theta(y^{(i)}x^{(i)}) \in [0, 1]$，所以$h_\theta(y^{(i)}x^{(i)})(1 - h_\theta(y^{(i)}x^{(i)}) \geq 0$，从而

$$z^T H z = \sum_{i=1}^m t_i^2 h_\theta(y^{(i)}x^{(i)})(1 - h_\theta(y^{(i)}x^{(i)}) \geq 0$$

从而H为半正定矩阵。

(b)(c)

这里解释下计算步骤，第一步是读取数据并增加一个截距项，由以下两个函数完成。

```
%matplotlib inline
import numpy as np
#import matplotlib as mpl
#mpl.use('Agg')
import matplotlib.pyplot as plt
from numpy.linalg import inv
#from __future__ import division


def load_data():
    X = np.genfromtxt('logistic_x.txt')
    Y = np.genfromtxt('logistic_y.txt')
    return X, Y

#增加截距项
def add_intercept(X_):
    m, n = X_.shape
    X = np.zeros((m, n + 1))
    ################
    ones = np.ones((m, 1))
    X = np.append(ones, X_, axis = 1)
    ################
    return X
```

第二步是利用刚刚的公式计算梯度以及$Hessian$矩阵。

```
#利用之前所述的公式计算
def calc_grad(X, Y, theta):
    m, n = X.shape
    grad = np.zeros(theta.shape)

    ##############
    Y_ = Y.reshape([-1, 1])
    d1 = (X*Y_).dot(theta)
    h = 1 / (1 + np.exp(-d1))
    S = (1 - h) * Y
    grad = -1/m * (X.T).dot(S)

    ##############

    return grad

def calc_hessian(X, Y, theta):
    m, n = X.shape
    H = np.zeros((n, n))

    ##############
    Y = Y.reshape([-1, 1])
    d1 = (X*Y).dot(theta)
    h = 1 / (1 + np.exp(-d1))
    S = np.diag(h * (1-h))
    H = X.T.dot(S).dot(X)

    #############

    return H
```

这里还有两个辅助的函数，分别是计算$J(\theta)$和作图。

```
def calc_loss(X, Y, theta):
    m, n = X.shape
    loss = 0.

    ###########
    Y = Y.reshape([-1, 1])
    d1 = (X*Y).dot(theta)
    h = 1 / (1 + np.exp(-d1))
    loss = -1/m * np.sum(np.log(h))

    ###########

    return loss

def plot(X, Y, theta):
    #plt.figure()

    ############
    x1 = X[Y>0][:, 1]
```

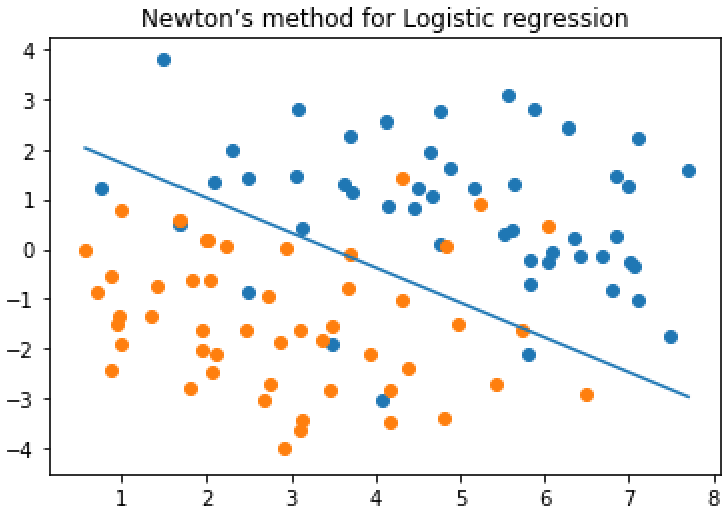
```
    y1 = X[Y>0][:, 2]
    x2 = X[Y<0][:, 1]
    y2 = X[Y<0][:, 2]
    #计算系数
    theta = logistic_regression(X, Y)
    Min = np.min(X[:, 1])
    Max = np.max(X[:, 1])
    x = np.array([Min, Max])
    y = -(theta[0] + theta[1]*x)/theta[2]
    plt.scatter(x1, y1)
    plt.scatter(x2, y2)
    plt.plot(x, y)
    plt.title('Newton's method for Logistic regression')
    ############

    plt.savefig('ps1q1c.png')
    return
```

最重要的一步就是利用如下公式迭代计算：

$$\theta = \theta - H^{-1}\nabla J(\theta)$$

```
def logistic_regression(X, Y):
    m, n = X.shape
    theta = np.zeros(n)

    ############
    H = calc_hessian(X, Y, theta)
    grad = calc_grad(X, Y, theta)
    theta -= inv(H).dot(grad)
    ############

    return theta
```

```
X_, Y = load_data()
X = add_intercept(X_)
theta = logistic_regression(X, Y)
plot(X, Y, theta)
```



全部代码可以查看my_logistic.py这个文件。

2.Poisson regression and the exponential family

(a)

$$p(y;\lambda)=\frac{e^{-\lambda}\lambda^y}{y!}=\frac{1}{y!}e^{y\log\lambda-\lambda}$$

对比指数族的形式

$$p(y;\eta)=b(y)\exp(\eta^TT(y)-a(\eta))$$

可得

$$b(y)=\frac{1}{y!},\eta=\log\lambda,T(y)=y,a(\eta)=\lambda=e^\eta$$

所以泊松分布为指数族

(b)我们来计算$g(\eta)=E[T(y);\eta]$

$$E[T(y);\eta]=E[y;\eta]=\lambda=e^\eta$$

(c)根据GLM的性质可知$\eta=\theta^Tx$，那么$\lambda=e^\eta=e^{\theta^Tx}$

计算对数似然函数

$$\begin{aligned}
l&=\log p(y^{(i)}|x^{(i)};\theta)\\
&=\log(\frac{e^{-\lambda}\lambda^{y^{(i)}}}{y^{(i)}!})\\
&=y^{(i)}\log\lambda-\lambda-\log(y^{(i)}!)\\
&=y^{(i)}\theta^Tx^{(i)}-e^{\theta^Tx^{(i)}}-\log(y^{(i)}!)
\end{aligned}$$

关于θ_j求偏导可得

$$\frac{\partial l}{\partial \theta_j} = y^{(i)} x_j^{(i)} - e^{\theta^T x^{(i)}} x_j = (y^{(i)} - e^{\theta^T x^{(i)}}) x_j$$

此处求最大值，用随机梯度上升法，更新规则为

$$\theta_j = \theta_j + (y^{(i)} - e^{\theta^T x^{(i)}}) x_j = \theta_j - (e^{\theta^T x^{(i)}} - y^{(i)}) x_j$$

(d)$T(y) = y$，所以

$$p(y;\eta) = b(y)\exp(\eta^T T(y) - a(\eta)) = b(y)\exp(\eta^T y - a(\eta))$$

$$E[T(y);\eta] = E[y;\eta]$$

$$\begin{aligned} l &= \log p(y|X;\theta) \\ &= \log\Big(b(y)\exp(\eta^T y - a(\eta))\Big) \\ &= \eta^T y - a(\eta) + \log b(y) \end{aligned}$$

因为$\eta = \theta^T x$，所以

$$\frac{\partial l}{\partial \theta_j} = y x_j - \frac{\partial a(\eta)}{\partial \eta}\frac{\partial \eta}{\partial \theta_j} = (y - \frac{\partial a(\eta)}{\partial \eta}) x_j$$

接下来只要证明$\frac{\partial a(\eta)}{\partial \eta} = h(x) = E[y;\eta]$即可，利用$p(y;\eta)$为概率密度函数

$$\begin{gathered} \int_{-\infty}^{+\infty} b(y)\exp(\eta^T y - a(\eta)) dy = 1 \\ \int_{-\infty}^{+\infty} b(y)\exp(\eta^T y) dy = \exp(a(\eta)) \\ \text{两边关于}\eta\text{求偏导可得} \\ \int_{-\infty}^{+\infty} y b(y)\exp(\eta^T y)) dy = \exp(a(\eta))\frac{\partial a(\eta)}{\partial \eta} \\ \frac{\partial a(\eta)}{\partial \eta} = \int_{-\infty}^{+\infty} y b(y)\exp(\eta^T y - a(\eta)) dy = E[y;\eta] \end{gathered}$$

所以

$$\frac{\partial l}{\partial \theta_j} = (y - h(x)) x_j$$

从而梯度上升法的更新规则为

$$\theta_j = \theta_j + \alpha(y - h(x)) x_j = \theta_j - \alpha(h(x) - y) x_j$$

3.Gaussian discriminant analysis

(a)先计算$P(x)$

$$
\begin{aligned}
P(x) &= P(y=1)P(x|y=1) + P(y=-1)P(x|y=-1) \\
&= \phi \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big) + (1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)
\end{aligned}
$$

利用贝叶斯公式计算$P(y|x)$，分$y=1, y=-1$计算

$$
\begin{aligned}
P(y|x) &= \frac{P(x|y)P(y)}{P(x)} \\
&= \frac{P(x|y)P(y)}{\phi \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big) + (1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)}
\end{aligned}
$$

所以

$$
\begin{aligned}
P(y=1|x) &= \frac{P(x|y=1)P(y=1)}{\phi \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big) + (1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)} \\
&= \frac{\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big)\phi}{\phi \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big) + (1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)} \\
&= \frac{1}{1+\frac{1-\phi}{\phi}\exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1}) + \frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big)} \\
P(y=-1|x) &= \frac{P(x|y=-1)P(y=-1)}{\phi \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big) + (1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)} \\
&= \frac{(1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)}{\phi \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\Big) + (1-\phi)\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)} \\
&= \frac{1}{1+\frac{\phi}{1-\phi}\exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) + \frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)}
\end{aligned}
$$

可以看到，指数部分都有一样的式子，现在计算这个式子

$$
\begin{aligned}
-\frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1}) + \frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) &= \frac{1}{2}\Big(x^T\Sigma^{-1}x - 2\mu_1^T\Sigma^{-1}x + \mu_1^T\Sigma^{-1}\mu_1 - x^T\Sigma^{-1}x + 2\mu_{-1}^T\Sigma^{-1}x - \mu_{-1}^T\Sigma^{-1}\mu_{-1}\Big) \\
&= \frac{1}{2}\Big(2(\mu_{-1}^T\Sigma^{-1} - \mu_1^T\Sigma^{-1})x + \mu_1^T\Sigma^{-1}\mu_1 - \mu_{-1}^T\Sigma^{-1}\mu_{-1}\Big) \\
&= (\mu_{-1}^T\Sigma^{-1} - \mu_1^T\Sigma^{-1})x + \frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1 - \mu_{-1}^T\Sigma^{-1}\mu_{-1})
\end{aligned}
$$

所以

$$
\begin{aligned}
P(y=1|x) &= \frac{1}{1+\frac{1-\phi}{\phi}\exp\Big((\mu_{-1}^T\Sigma^{-1} - \mu_1^T\Sigma^{-1})x + \frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1 - \mu_{-1}^T\Sigma^{-1}\mu_{-1})\Big)} \\
&= \frac{1}{1+\exp\Big((\mu_{-1}^T\Sigma^{-1} - \mu_1^T\Sigma^{-1})x + \frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1 - \mu_{-1}^T\Sigma^{-1}\mu_{-1}) + \ln(\frac{1-\phi}{\phi})\Big)} \\
P(y=-1|x) &= \frac{1}{1+\frac{\phi}{1-\phi}\exp\Big(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) + \frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})\Big)} \\
&= \frac{1}{1+\exp\Big(-(\mu_{-1}^T\Sigma^{-1} - \mu_1^T\Sigma^{-1})x - \frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1 - \mu_{-1}^T\Sigma^{-1}\mu_{-1}) - \ln(\frac{1-\phi}{\phi})\Big)}
\end{aligned}
$$

综合两式，$P(y|x)$可以写为

$$
\begin{aligned}
P(y|x) &= \frac{1}{1+\exp\Big(y\Big((\mu_{-1}^T\Sigma^{-1}-\mu_1^T\Sigma^{-1})x+\frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1-\mu_{-1}^T\Sigma^{-1}\mu_{-1})+\ln(\frac{1-\phi}{\phi})\Big)\Big)}\\
&= \frac{1}{1+\exp\Big(-y\Big((\mu_1^T\Sigma^{-1}-\mu_{-1}^T\Sigma^{-1})x-\frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1-\mu_{-1}^T\Sigma^{-1}\mu_{-1})-\ln(\frac{1-\phi}{\phi})\Big)\Big)}
\end{aligned}
$$

令

$$
\begin{aligned}
\theta &= (\mu_1^T\Sigma^{-1}-\mu_{-1}^T\Sigma^{-1})^T=\Sigma^{-1}(\mu_1-\mu_{-1})\\
\theta_0 &= -\frac{1}{2}(\mu_1^T\Sigma^{-1}\mu_1-\mu_{-1}^T\Sigma^{-1}\mu_{-1})-\ln(\frac{1-\phi}{\phi})
\end{aligned}
$$

从而

$$
p(y|x;\varphi,\Sigma,\mu_{-1},\mu_1)=\frac{1}{1+\exp(-y(\theta^Tx+\theta_0))}
$$

(b)(c)

(c)是(b)的一般情形，所以直接处理(c)

先观察$P(x|y)$的形式，可以得到如下公式

$$
P(x|y)=\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}}\exp\Big(-\frac{1}{2}(x-\mu_y)^T\Sigma^{-1}(x-\mu_y)\Big)
$$

接着计算$\log P(x,y)$

$$
\begin{aligned}
\log P(x,y) &= \log P(x|y)P(y)\\
&= \log\Big(\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}}\exp\Big(-\frac{1}{2}(x-\mu_y)^T\Sigma^{-1}(x-\mu_y)\Big)\phi^{1\{y=1\}}(1-\phi)^{1\{y=-1\}}\Big)\\
&= \log\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}}-\frac{1}{2}(x-\mu_y)^T\Sigma^{-1}(x-\mu_y)+1\{y=1\}\log\phi+1\{y=-1\}\log(1-\phi)
\end{aligned}
$$

对数似然函数为

$$
\begin{aligned}
\ell(\varphi,\mu_{-1},\mu_1,\Sigma) &= \log\prod_{i=1}^m p(x^{(i)},y^{(i)};\varphi,\mu_{-1},\mu_1,\Sigma)\\
&= \sum_{i=1}^m \log p(x^{(i)},y^{(i)};\varphi,\mu_{-1},\mu_1,\Sigma)\\
&= \sum_{i=1}^m\Big(\log\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}}-\frac{1}{2}(x^{(i)}-\mu_{y^{(i)}})^T\Sigma^{-1}(x^{(i)}-\mu_{y^{(i)}})+1\{y^{(i)}=1\}\log\phi+1\{y^{(i)}=-1\}\log(1-\phi)\Big)
\end{aligned}
$$

关于ϕ求梯度

$$\frac{\partial \ell}{\partial \phi} = \sum_{i=1}^{m}\Big(\frac{1\{y^{(i)}=1\}}{\phi} - \frac{1\{y^{(i)}=-1\}}{1-\phi}\Big) = 0$$

$$\sum_{i=1}^{m} 1\{y^{(i)}=1\}(1-\phi) - 1\{y^{(i)}=-1\}\phi = 0$$

$$\sum_{i=1}^{m} 1\{y^{(i)}=1\} = m\phi$$

$$\phi = \frac{1}{m}\sum_{i=1}^{m} 1\{y^{(i)}=1\}$$

关于μ_1,μ_{-1}求梯度

$$\nabla_{\mu_1}\ell = -\sum_{i=1}^{m}\Sigma^{-1}(x^{(i)}-\mu_{y^{(i)}})1\{y^{(i)}=1\} = 0$$

$$\sum_{i=1}^{m}(x^{(i)}-\mu_1)1\{y^{(i)}=1\} = 0$$

$$\mu_1 = \frac{\sum_{i=1}^{m}1\{y^{(i)}=1\}x^{(i)}}{\sum_{i=1}^{m}1\{y^{(i)}=1\}}$$

$$\nabla_{\mu_{-1}}\ell = -\sum_{i=1}^{m}\Sigma^{-1}(x^{(i)}-\mu_{y^{(i)}})1\{y^{(i)}=-1\} = 0$$

$$\sum_{i=1}^{m}(x^{(i)}-\mu_{-1})1\{y^{(i)}=-1\} = 0$$

$$\mu_{-1} = \frac{\sum_{i=1}^{m}1\{y^{(i)}=-1\}x^{(i)}}{\sum_{i=1}^{m}1\{y^{(i)}=-1\}}$$

求$\sum$的时候利用一些技巧性，我们不求$\sum$的极大似然估计，而是求$\sum^{-1}$的极大似然估计，然后再求出$\sum$的极大似然估计，利用如下两个式子

$$\nabla_A \det|A| = \det|A|(A^{-1})^T$$
$$\nabla_A(x^TAy) = \nabla_A \mathrm{trace}(x^TAy) = xy^T$$

那么

$$\nabla_{\sum^{-1}}\ell = \nabla_{\sum^{-1}}\Big(\frac{m}{2}\log\Big|\sum^{-1}\Big|\Big) - \frac{1}{2}\nabla_{\sum^{-1}}\sum_{i=1}^{m}(x^{(i)}-\mu_y^{(i)})^T\Sigma^{-1}(x^{(i)}-\mu_y^{(i)}) = 0$$

$$\frac{m}{2}\frac{1}{\Big|\sum^{-1}\Big|}\Big|\sum^{-1}\Big|\sum - \frac{1}{2}\sum_{i=1}^{m}(x^{(i)}-\mu_y^{(i)})(x^{(i)}-\mu_y^{(i)})^T = 0$$

$$\sum = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)}-\mu_y^{(i)})(x^{(i)}-\mu_y^{(i)})^T$$

所以结论成立。

4.Linear invariance of optimization algorithms

(a)我们计算$\nabla_z g(z),\nabla_z^2 g(z)$。

先计算$\nabla_z g(z)$,

$$
\begin{aligned}
\frac{\partial g(z)}{\partial z_i} &= \sum_{k=1}^{n}\frac{\partial f(Az)}{\partial (Az)_k}\frac{\partial (Az)_k}{\partial z_i}\\
&= \sum_{k=1}^{n}\frac{\partial f(Az)}{\partial x_k}\frac{\partial (Az)_k}{\partial z_i}\\
&= \sum_{k=1}^{n}\frac{\partial f(Az)}{\partial x_k}A_{ki}\\
&= (A^T)_i \nabla_x f(Az)\\
&(A^T)_i\text{表示}A^T\text{的第}i\text{行}
\end{aligned}
$$

所以

$$
\nabla_z g(z) = A^T\nabla_x f(Az)
$$

接着计算$\nabla_z^2 g(z)$

$$
\begin{aligned}
\frac{\partial^2 g(z)}{\partial z_j\partial z_i} &= \frac{\partial\left(\sum_{k=1}^{n}\frac{\partial f(Az)}{\partial x_k}A_{ki}\right)}{\partial z_j}\\
&= \sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial^2 f(Az)}{\partial (Az)_l\partial x_k}\frac{\partial (Az)_l}{\partial x_j}A_{ki}\\
&= \sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial^2 f(Az)}{\partial (Az)_l\partial x_k}\frac{\partial (Az)_l}{\partial x_j}A_{ki}\\
&= \sum_{k=1}^{n}\sum_{l=1}^{n}\frac{\partial^2 f(Az)}{\partial x_l\partial x_k}A_{lj}A_{ki}
\end{aligned}
$$

从而

$$
\nabla_z^2 g(z) = A^T\nabla_x^2 f(Az)A
$$

接着利用数学归纳法来证明结论。

$n=0$时，

$$
z^{(0)} = A^{-1}x^{(0)} = 0
$$

所以$n=0$时结论成立。假设$n\le i$时，$z^{(n)} = A^{-1}x^{(n)}$，那么$n=i+1$时

$$
\begin{aligned}
z^{(i+1)} &= z^{(i)} - (\nabla_z^2 g(z^{(i)}))^{-1}\nabla_z g(z)\\
&= A^{-1}x^{(i)} - A^{-1}(\nabla_x^2 f(Az^{(i)}))^{-1}(A^T)^{-1}A^T\nabla_x f(Az^{(i)})\\
&= A^{-1}x^{(i)} - A^{-1}(\nabla_x^2 f(Az^{(i)}))^{-1}\nabla_x f(Az^{(i)})\\
&= A^{-1}(x^{(i)} - (\nabla_x^2 f(Az^{(i)}))^{-1}\nabla_x f(Az^{(i)}))\\
&= A^{-1}(x^{(i)} - (\nabla_x^2 f(x^{(i)}))^{-1}\nabla_x f(x^{(i)}))\\
&= A^{-1}x^{(i+1)}
\end{aligned}
$$

其中倒数第二步是因为$x^{(i)} = Az^{(i)}$，所以$n=i+1$时结论成立，从而牛顿法满足invariant to linear reparameterizations

(b)对于梯度下降法， 继续利用

$$
\nabla_z g(z) = A^T\nabla_x f(Az)
$$

假设$z^{(i)}=A^{-1}x^{(i)}$，那么

$$\begin{aligned}z^{(i+1)}&=z^{(i)}-\alpha\nabla_z g(z)\\&=A^{-1}x^{(i)}-\alpha A^T\nabla_x f(Az)\\&=A^{-1}x^{(i)}-\alpha A^T\nabla_x f(x^{(i)})\end{aligned}$$

但是

$$\begin{aligned}x^{(i+1)}&=x^{(i)}-\alpha\nabla_x f(x^{(i)})\\A^{-1}x^{(i+1)}&=A^{-1}x^{(i)}-\alpha A^{-1}\nabla_x f(x^{(i)})\end{aligned}$$

所以$z^{(i+1)}$与$A^{-1}x^{(i+1)}$不相等，从而梯度下降法不满足invariant to linear reparameterizations

5.Regression for denoising quasar spectra

(a)

(i)

$$J(\theta)=\frac{1}{2}\sum_{i=1}^{m}w^{(i)}\left(\theta^Tx^{(i)}-y^{(i)}\right)^2$$

记

$$\begin{aligned}X&=[x^{(1)},\ldots,x^{(m)}]^T\\y&=[y^{(1)},\ldots,y^{(m)}]^T\\W&=\frac{1}{2}\text{diag}\{w^{(1)},\ldots,w^{(m)}\}\end{aligned}$$

那么

$$J(\theta)=(X\theta-y)^TW(X\theta-y)$$

(ii)

$$\begin{aligned}J(\theta)&=(X\theta-y)^TW(X\theta-y)\\&=\theta^TX^TWX\theta-2y^TW^TX\theta+y^Ty\\\nabla J(\theta)&=2X^TWX\theta-2X^TWy=0\\\theta&=(X^TWX)^{-1}X^TWy\end{aligned}$$

(iii)

$$p(y^{(i)}|x^{(i)};\theta)=\frac{1}{\sqrt{2\pi}\sigma^{(i)}}\exp\Big(-\frac{(y^{(i)}-\theta^Tx^{(i)})^2}{2(\sigma^{(i)})^2}\Big)^2$$

概率似然函数为

$$\prod_{i=1}^{m}\frac{1}{\sqrt{2\pi}\sigma^{(i)}}\exp\Big(-\frac{(y^{(i)}-\theta^Tx^{(i)})^2}{2(\sigma^{(i)})^2}\Big)^2=\Big(\prod_{i=1}^{m}\frac{1}{\sqrt{2\pi}\sigma^{(i)}}\Big)\exp\Big(-\sum_{i=1}^{m}\frac{(y^{(i)}-\theta^Tx^{(i)})^2}{2(\sigma^{(i)})^2}\Big)^2$$

对于固定的$\sigma^{(i)}$，最大化这个概率似然函数等价于最小化

$$\frac{1}{2}\sum_{i=1}^{m}\frac{(y^{(i)}-\theta^T x^{(i)})^2}{(\sigma^{(i)})^2}$$

记$w^{(i)}=\frac{1}{(\sigma^{(i)})^2}$，这个是式子可以转化为

$$\frac{1}{2}\sum_{i=1}^{m}w^{(i)}(y^{(i)}-\theta^T x^{(i)})^2$$

(b)

(i)

第一步还是读取数据以及增加截距。

```
%matplotlib inline
import numpy as np
#import matplotlib as mpl
#mpl.use('Agg')
import matplotlib.pyplot as plt
from numpy.linalg import inv

def load_data():
    train = np.genfromtxt('quasar_train.csv', skip_header=True, delimiter=',')
    test = np.genfromtxt('quasar_test.csv', skip_header=True, delimiter=',')
    wavelengths = np.genfromtxt('quasar_train.csv', skip_header=False, delimiter=',')[0]
    return train, test, wavelengths

def add_intercept(X_):
    X = None
    #####################
    X_ = X_.reshape((-1, 1))
    m, n = X_.shape
    ones = np.ones((m, 1))
    X = np.append(ones, X_, axis = 1)

    ###################
    return X
```

这一部分直接利用最小二乘法计算结果。

```python
#利用最小二乘公式
def LR_smooth(Y, X_):
    X = add_intercept(X_)
    Y = Y.reshape((-1, 1))
    yhat = np.zeros(Y.shape)
    theta = np.zeros(2)
    #####################
    theta = inv(X.T.dot(X)).dot(X.T).dot(Y)
    yhat = X.dot(theta)

    #####################
    return yhat, theta
```

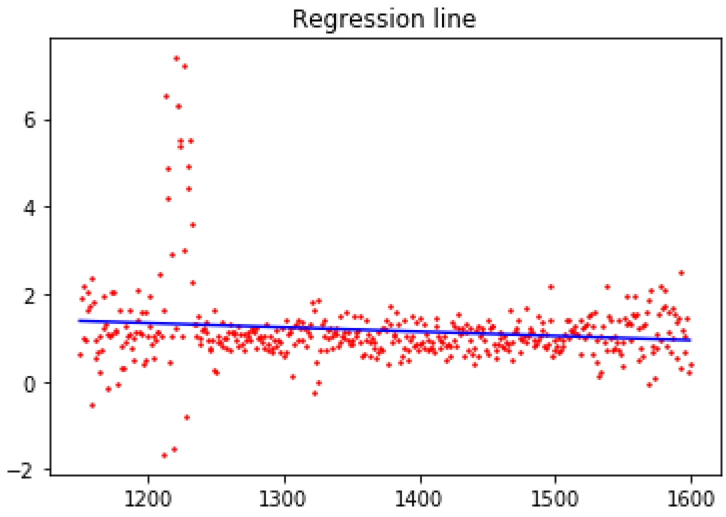
作图函数

```python
def plot_b(X, raw_Y, Ys, desc, filename):
    plt.figure()
    ############
    for i in range(len(Ys)):
        plt.scatter(X, raw_Y, c='red', s=2, label='raw_data')
        plt.plot(X, Ys[i], c='blue', label='Regression line')
        plt.title(desc[i])
        plt.show()

    ############
    plt.savefig(filename)
```

产生结果

```python
raw_train, raw_test, wavelengths = load_data()

## Part b.i
lr_est, theta = LR_smooth(raw_train[0], wavelengths)
print('Part b.i) Theta=[%.4f, %.4f]' % (theta[0], theta[1]))
plot_b(wavelengths, raw_train[0], [lr_est], ['Regression line'], 'ps1q5b1.png')
```

```
Part b.i) Theta=[2.5134, -0.0010]
```

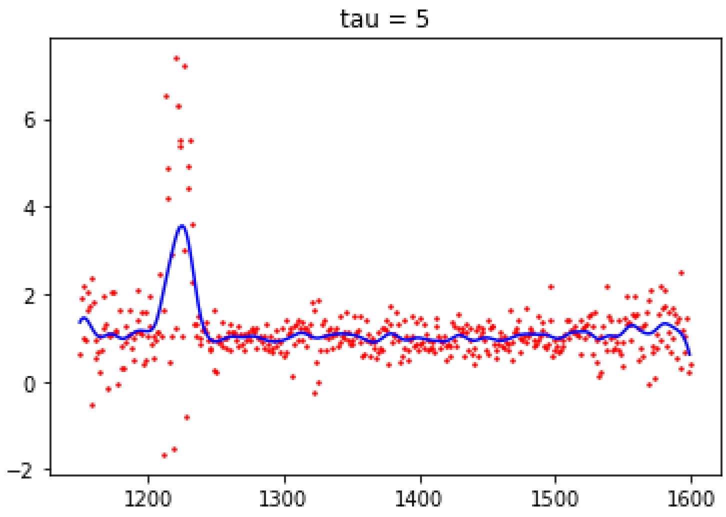


(ii)利用a中的公式$\theta = (X^TWX)^{-1}X^TWy$计算

```
def LWR_smooth(spectrum, wavelengths, tau):
    smooth_spectrum = np.array([])
    ###############
    X = add_intercept(wavelengths)
    Y = spectrum.reshape((-1, 1))
    for i in range(len(wavelengths)):
        w = np.exp(-(wavelengths - wavelengths[i])**2 / (2*tau**2))
        W = np.diag(w)
        theta = inv(X.T.dot(W).dot(X)).dot(X.T).dot(W).dot(Y)
        yhat = theta.T.dot(X[i])
        smooth_spectrum = np.append(smooth_spectrum, yhat)
    ###############
    return smooth_spectrum
```

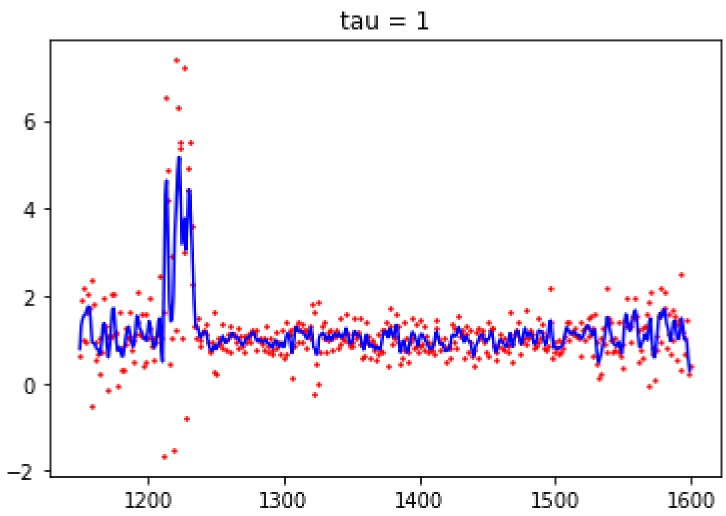
计算结果

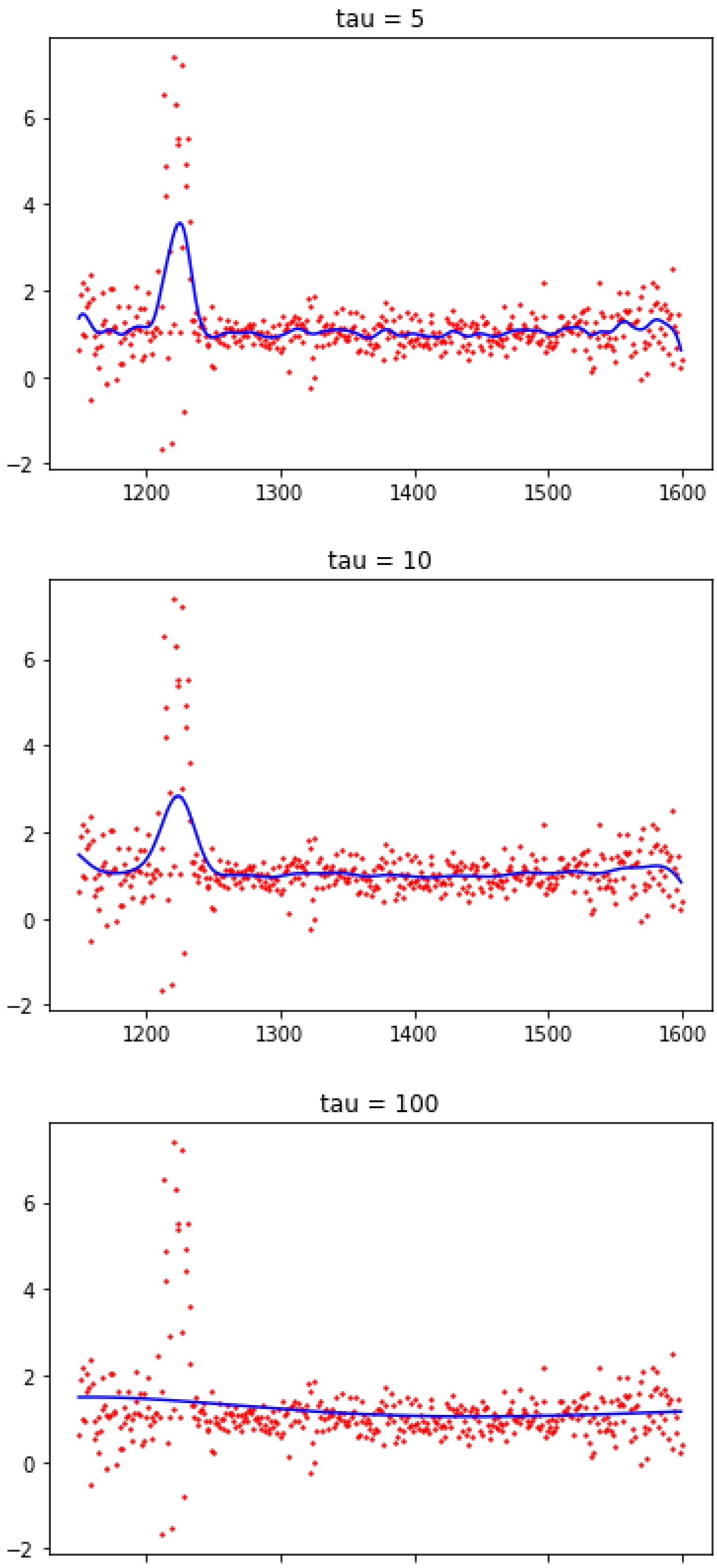
```
## Part b.ii
lwr_est_5 = LWR_smooth(raw_train[0], wavelengths, 5)
plot_b(wavelengths, raw_train[0], [lwr_est_5], ['tau = 5'], 'ps1q5b2.png')
```

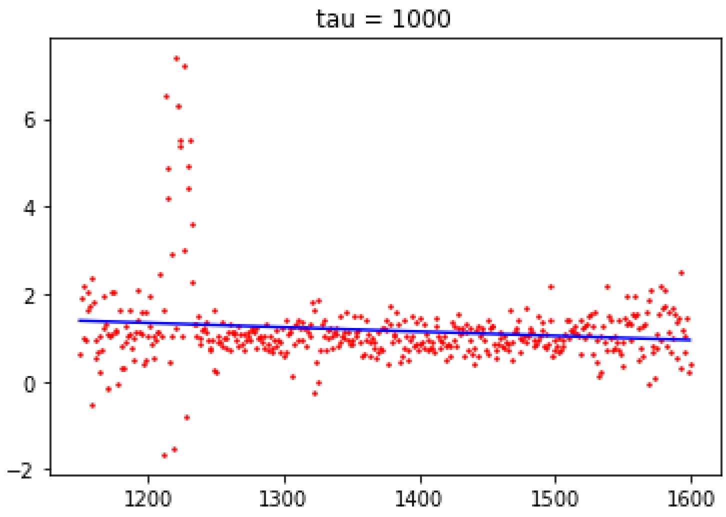


对不同的参数作图。

```
### Part b.iii
lwr_est_1 = LWR_smooth(raw_train[0], wavelengths, 1)
lwr_est_10 = LWR_smooth(raw_train[0], wavelengths, 10)
lwr_est_100 = LWR_smooth(raw_train[0], wavelengths, 100)
lwr_est_1000 = LWR_smooth(raw_train[0], wavelengths, 1000)
plot_b(wavelengths, raw_train[0],
       [lwr_est_1, lwr_est_5, lwr_est_10, lwr_est_100, lwr_est_1000],
       ['tau = 1', 'tau = 5', 'tau = 10', 'tau = 100', 'tau = 1000'],
       'ps1q5b3.png')
```




tau = 5
tau = 10
tau = 100



(c)

(i)

第一步是利用局部加权回归来使得数据更平滑一些。

```
def smooth_data(raw, wavelengths, tau):
    smooth = None
    ################
    smooth = []
    for spectrum in raw:
        smooth.append(LWR_smooth(spectrum, wavelengths, tau))
    ################
    return np.array(smooth)

smooth_train, smooth_test = [smooth_data(raw, wavelengths, 5) for raw in [raw_train, raw_test]]
```

(ii) 这部分比较难懂，详细解释下各个步骤，第一步将数据分为左边和右边，波长小于1200的为left，大于1300的为right，利用如下函数完成这部分工作。

```
def split(full, wavelengths):
    left, right = None, None
    ###############
    indexl = np.argwhere(wavelengths == 1200)[0][0]
    indexr = np.argwhere(wavelengths == 1300)[0][0]
    left = full[:, :indexl]
    right = full[:, indexr:]
    ###############
    return left, right
```

第二步要计算距离，定义如下函数

```
def dist(a, b):
    dist = 0
    ################
    dist = ((a - b)**2).sum()
    ################
    return dist
```

```
#### Part c.ii
left_train, right_train = split(smooth_train, wavelengths)
left_test, right_test = split(smooth_test, wavelengths)
```

最后一步是最复杂的，首先计算距离，这里的距离定义为

$$d(f_1, f_2) = \sum_i (f_1(\lambda_i) - f_2(\lambda_i))^2$$

对于此题来说，$f_1(\lambda), f_2(\lambda)$分别对应了测试数据以及训练数据，利用下式计算距离矩阵。

```
d = (right_train - right_test)**2

#求和
d1 = d.sum(axis=1)
```

然后要找到距离最近的k个点，这里为3个点，我的思路是先对数据进行排序，然后找到前三个数据的索引

```
#找到排名前3的作为neighb_k(f_right)
tempd = d1.copy()
tempd.sort()
#找到索引
index = (d1==tempd[0])|(d1==tempd[1])|(d1==tempd[2])
```

接着计算h，为距离的最大值，根据题目中的公式对数据进行转换

```
h = d1.max()
d1 = d1/h
```

最后一步根据kernel以及题目中的公式计算即可

```
d1 = 1 - d1
#求lefthat
a = (d1[index].dot(left_train[index]))
b = d1[index].sum()

lefthat = a/b
```

以上全部综合起来就是如下函数：

```
def func_reg(left_train, right_train, right_test):
    m, n = left_train.shape
    #m=200,n=50
    lefthat = np.zeros(n)
    ###########################
    #right_train 200*300
    #right_test  1*300
    #left_train  200*50
    #求题目中的d(f1,f2),先求每个点的距离,200*300矩阵
    d = (right_train - right_test)**2
    #按照行求和200*1
    d1 = d.sum(axis=1)
    #找到排名前3的作为neighb_k(f_right)
    tempd = d1.copy()
    tempd.sort()
    #找到索引
    index = (d1==tempd[0])|(d1==tempd[1])|(d1==tempd[2])
    #h为d1中的最大值
    h = d1.max()
    d1 = d1/h
    #ker (1-t)
    d1 = 1 - d1
    #求lefthat
    a = (d1[index].dot(left_train[index]))
    b = d1[index].sum()

    lefthat = a/b
    ###########################
    return lefthat
```

作图函数

```
#将左边右边区分开来,左边<1200,右边>=1300
def plot_c(Yhat, Y, X, filename):
    plt.figure()
    ############
    plt.plot(X[:50],Yhat)
    plt.plot(X,Y)
    plt.show()
    #############
    plt.savefig(filename)
    return
```

产生结果

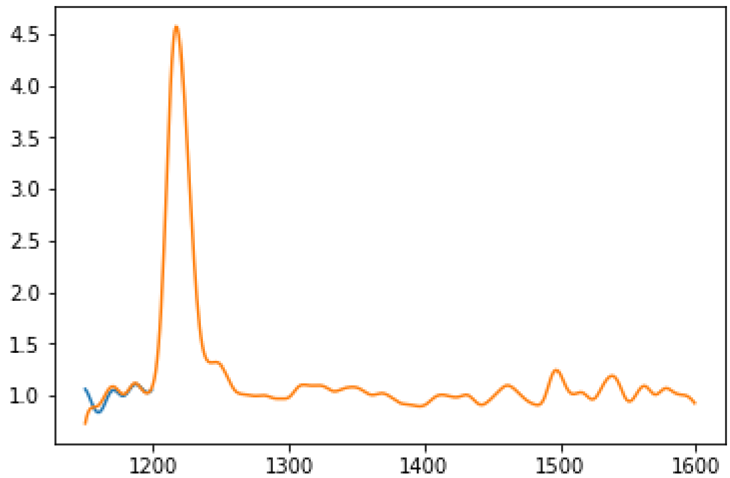
```
#### Part c.ii
left_train, right_train = split(smooth_train, wavelengths)
left_test, right_test = split(smooth_test, wavelengths)

train_errors = [dist(left, func_reg(left_train, right_train, right)) for left, right in zip(left_train, right_train)]
print('Part c.ii) Training error: %.4f' % np.mean(train_errors))
```

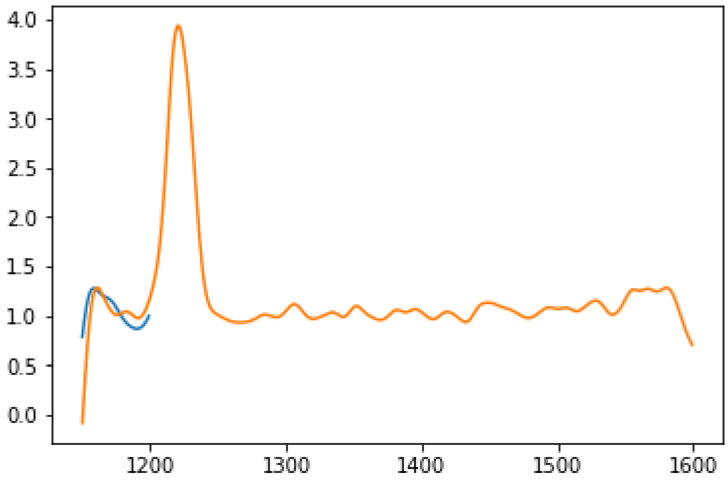
```
Part c.ii) Training error: 1.0664
```

(iii)

```
### Part c.iii
test_errors = [dist(left, func_reg(left_train, right_train, right)) for left, right in zip(left_test, right_test)]
print('Part c.iii) Test error: %.4f' % np.mean(test_errors))

left_1 = func_reg(left_train, right_train, right_test[0])
plot_c(left_1, smooth_test[0], wavelengths, 'ps1q5c3_1.png')
left_6 = func_reg(left_train, right_train, right_test[5])
plot_c(left_6, smooth_test[5], wavelengths, 'ps1q5c3_6.png')
```

```
Part c.iii) Test error: 2.7100
```





全部代码可以查看my_quasars.py这个文件。