CS 229, Fall 2018

Problem Set #1 Solutions: Supervised Learning → Logistic Regression

$$Y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{pmatrix}_{m\times 1} \qquad X = \begin{pmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)} \\ & \vdots & & \\ x_1^{(m)} & x_2^{(m)} & \cdots & x_n^{(m)} \end{pmatrix}_{m\times n} \qquad \theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{pmatrix}$$

1.

(a)

$$\begin{aligned}
\frac{\partial J(\theta)}{\partial \theta_j} &= -\frac{1}{m}\sum_{i=1}^{m}\Big(y^{(i)}\frac{g(\theta^T x^{(i)})[1-g(\theta^T x^{(i)})]}{g(\theta^T x^{(i)})}x_j^{(i)} - (1-y^{(i)})\frac{g(\theta^T x^{(i)})[1-g(\theta^T x^{(i)})]}{1-g(\theta^T x^{(i)})}x_j^{(i)}\Big) \\
&= -\frac{1}{m}\sum_{i=1}^{m}\Big(y^{(i)}[1-g(\underbrace{\theta^T x^{(i)}}_{X\theta})]x_j^{(i)} - (1-y^{(i)})g(\theta^T x^{(i)})x_j^{(i)}\Big) \\
&= \frac{1}{m}\sum_{i=1}^{m}[g(\theta^T x^{(i)}) - y^{(i)}]x_j^{(i)}
\end{aligned}$$

$$X^T = \begin{pmatrix} x_1^{(1)} & \cdots & x_1^{(m)} \\ \vdots & \ddots & \vdots \\ x_n^{(1)} & \cdots & x_n^{(m)} \end{pmatrix}$$

$$\nabla_\theta J(\theta) = \frac{1}{m}X^T(g(X\theta) - Y)$$

$$x_{jk} = (x_j^{(1)}\ x_j^{(2)}\ \cdots\ x_j^{(m)}) \begin{pmatrix} x_k^{(1)} \\ x_k^{(2)} \\ \vdots \\ x_k^{(m)} \end{pmatrix} = \sum_{i=1}^{m} x_j^{(i)} x_k^{(i)}$$

$$\frac{\partial}{\partial\theta_k}\cdot\frac{\partial J(\theta)}{\partial\theta_j} = \frac{\partial}{\partial\theta_k}\Big(\frac{1}{m}\sum_{i=1}^{m}[g(\theta^T x^{(i)}) - y^{(i)}]x_j^{(i)}\Big) = \frac{\partial}{\partial\theta_k}\Big(\frac{1}{m}\sum_{i=1}^{m}[g(\theta^T x^{(i)})]x_j^{(i)}\Big)$$

$$H_{jk} = \frac{\partial^2 J(\theta)}{\partial\theta_j\partial\theta_k} = \frac{1}{m}\sum_{i=1}^{m} g(\underbrace{\theta^T x^{(i)}}_{X\theta})[1-g(\theta^T x^{(i)})]x_j^{(i)}x_k^{(i)}$$

$$\therefore \boxed{H = \frac{1}{m}[X^T\cdot g(X\theta)\cdot(1-g(X\theta))]X}$$

当j取1,…n时，k取1…n时，

$$X = \begin{pmatrix} x_1^{(1)} & \cdots & x_1^{(m)} \\ \vdots & & \vdots \\ x_n^{(1)} & \cdots & x_n^{(m)} \end{pmatrix}\begin{pmatrix} x_1^{(1)} & \cdots & x_n^{(1)} \\ x_1^{(2)} & & \vdots \\ \vdots & & \\ x_1^{(m)} & \cdots & x_n^{(m)} \end{pmatrix} = X^T\cdot X$$

n features

$$\begin{aligned}
z^T H z &= \frac{1}{m}\sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{n} g(\theta^T x^{(i)})[1-g(\theta^T x^{(i)})]x_j^{(i)}x_k^{(i)}z_j z_k \\
&= \frac{1}{m}\sum_{i=1}^{m} g(\theta^T x^{(i)})[1-g(\theta^T x^{(i)})][(x^{(i)})^T z]^2 \geq 0
\end{aligned}$$

(c)

分子分母同乘以 $\dfrac{1}{\exp\{-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\}\phi}$

$$\begin{aligned}
p(y=1|x) &= \frac{p(x|y=1)p(y=1)}{p(x|y=1)p(y=1) + p(x|y=0)p(y=0)} \\
&= \frac{\exp\{-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\}\phi}{\exp\{-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\}\phi + \exp\{-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)\}(1-\phi)} \\
&= \frac{1}{1+\exp\{\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) - \frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)\}\frac{1-\phi}{\phi}} \\
&= \frac{1}{1+\exp\{-[\underbrace{(\Sigma^{-1}(\mu_1-\mu_0))}_{\theta}{}^T x + \underbrace{\tfrac{1}{2}(\mu_0+\mu_1)^T\Sigma^{-1}(\mu_0-\mu_1) - \ln(\tfrac{1-\phi}{\phi})}_{\theta_0}]\}}
\end{aligned}$$

$$\theta = \Sigma^{-1}(\mu_1 - \mu_0)$$

$$\theta_0 = \frac{1}{2}(\mu_0+\mu_1)^T\Sigma^{-1}(\mu_0-\mu_1) - \ln(\frac{1-\phi}{\phi})$$

$$= \frac{1}{1+\exp(-(\theta^T x + \theta_0))}$$

(d)

To compute ϕ, μ_0 and μ_1, recall the log-likelihood:

$$
\begin{aligned}
\ell(\phi, \mu_0, \mu_1, \Sigma) &= \log \prod_{i=1}^{m} p(x^{(i)}, y^{(i)};\ \phi, \mu_0, \mu_1, \Sigma) \\
&= \log \prod_{i=1}^{m} p(x^{(i)} \mid y^{(i)};\ \mu_0, \mu_1, \Sigma)\, p(y^{(i)};\ \phi) \\
&= \log \prod_{i=1}^{m} \big(p(x^{(i)} \mid y^{(i)} = 1;\ \mu_0, \mu_1, \Sigma)\, p(y^{(i)} = 1;\ \phi)\big)^{1\{y^{(i)}=1\}} \big(p(x^{(i)} \mid y^{(i)} = 0;\ \mu_0, \mu_1, \Sigma)\, p(y^{(i)} = 0;\ \phi)\big)^{1\{y^{(i)}=0\}} \\
&= \sum_{i=1}^{m} 1\{y^{(i)} = 1\}\Big(-\frac{1}{2}(x^{(i)} - \mu_1)^T \Sigma^{-1} (x^{(i)} - \mu_1) + \log \phi\Big) + \sum_{i=1}^{m} 1\{y^{(i)} = 0\}\Big(-\frac{1}{2}(x^{(i)} - \mu_0)^T \Sigma^{-1} (x^{(i)} - \mu_0) + \log(1 - \phi)\Big) + C
\end{aligned}
$$

where C does not contain ϕ, μ_0 or μ_1.

Take derivative of ℓ w.r.t ϕ and set to 0:

$$
\begin{aligned}
\frac{\partial}{\partial \phi}\ell(\phi, \mu_0, \mu_1, \Sigma) &= \sum_{i=1}^{m} 1\{y^{(i)} = 1\}\frac{1}{\phi} + \big(m - \sum_{i=1}^{m} 1\{y^{(i)} = 1\}\big)\frac{1}{1 - \phi} \\
&= 0
\end{aligned}
$$

We have $\boxed{\phi = \frac{1}{m}\sum_{i=1}^{m} 1\{y^{(i)} = 1\}}$.

Also, take derivative of ℓ w.r.t μ_0 and set to 0:

$$
\begin{aligned}
\frac{\partial}{\partial \mu_0}\ell(\phi, \mu_0, \mu_1, \Sigma) &= \sum_{i=1}^{m} 1\{y^{(i)} = 0\}\Sigma^{-1}(x^{(i)} - \mu_0) \\
&= 0
\end{aligned}
$$

We can easily obtain that $\boxed{\mu_0 = \sum_{i=1}^{m} 1\{y^{(i)} = 0\}x^{(i)} / \sum_{i=1}^{m} 1\{y^{(i)} = 0\}}$. Similarly $\boxed{\mu_1 = \sum_{i=1}^{m} 1\{y^{(i)} = 1\}x^{(i)} / \sum_{i=1}^{m} 1\{y^{(i)} = 1\}}$.

To compute Σ, we need to simplify ℓ while maintaining Σ:

$$
\begin{aligned}
\ell(\phi, \mu_0, \mu_1, \Sigma) &= \log \prod_{i=1}^{m} p(x^{(i)} \mid y^{(i)};\ \mu_0, \mu_1, \Sigma)\, p(y^{(i)};\ \phi) \\
&= -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{m}(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1} (x^{(i)} - \mu_{y^{(i)}}) + C \\
&= -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{m} \operatorname{tr}\big((x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1} (x^{(i)} - \mu_{y^{(i)}})\big) + C \\
&= -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{m} \operatorname{tr}\big(\Sigma^{-1}(x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T\big) + C
\end{aligned}
$$

Since $n = 1$, i.e. $|\Sigma| = \sigma^2$, by taking derivative of ℓ w.r.t Σ and set to 0:

$$
\begin{aligned}
\frac{\partial}{\partial \Sigma}\ell(\phi, \mu_0, \mu_1, \Sigma) &= -\frac{m}{2\Sigma} + \frac{1}{2}\sum_{i=1}^{m}(x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-2} \\
&= 0
\end{aligned}
$$

We have: $\boxed{\Sigma = \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T}$.

In fact, even if $n \neq 1$, this maximum likelihood estimate still holds. Recall that:

$$
\begin{aligned}
\det(A^{-1}) &= \frac{1}{\det(A)} \\
\frac{\partial}{\partial A}\log|A| &= A^{-T}
\end{aligned}
$$

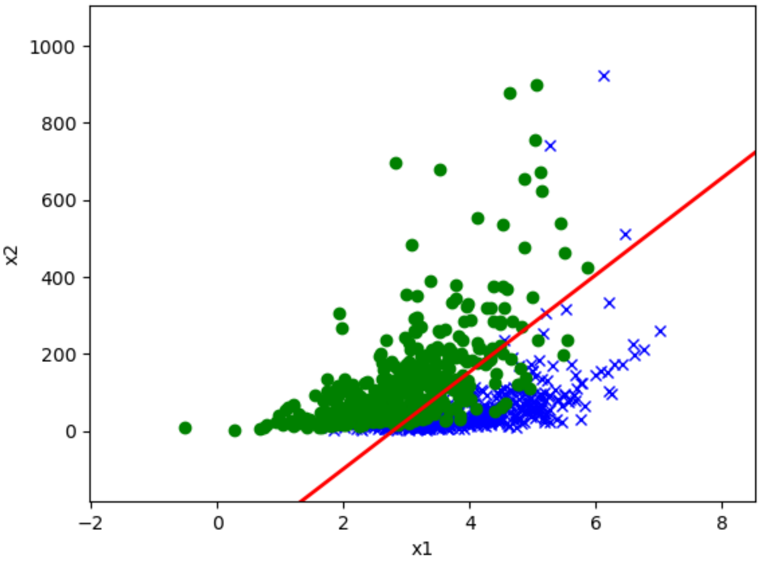
Simplify ℓ w.r.t Σ^{-1}:

$$
\begin{aligned}
\ell(\phi, \mu_0, \mu_1, \Sigma) &= -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{m}(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1} (x^{(i)} - \mu_{y^{(i)}}) + C \\
&= \frac{m}{2}\log|\Sigma^{-1}| - \frac{1}{2}\sum_{i=1}^{m}\Sigma^{-1}(x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T + C
\end{aligned}
$$

We can derive the same estimate by solving:

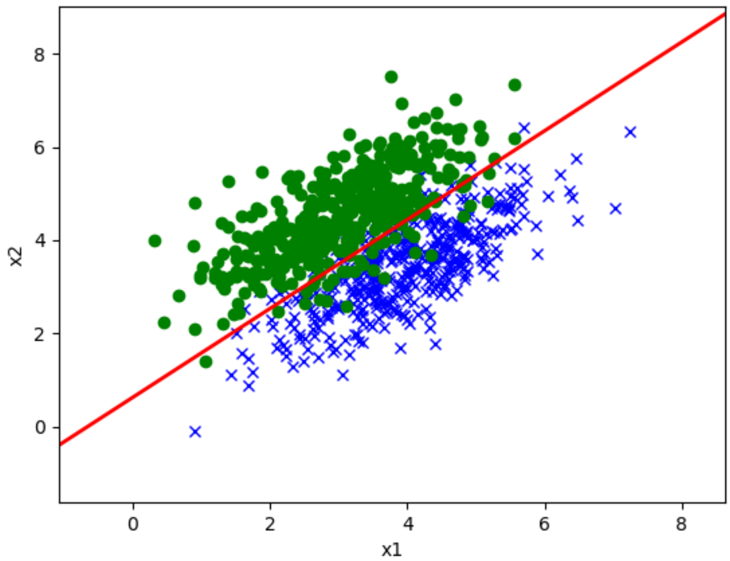
$$
\begin{aligned}
\frac{\partial}{\partial \Sigma^{-1}}\ell(\phi, \mu_0, \mu_1, \Sigma) &= \frac{m}{2}\Sigma - \frac{1}{2}\sum_{i=1}^{m}(x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T \\
&= 0
\end{aligned}
$$

logistic regression

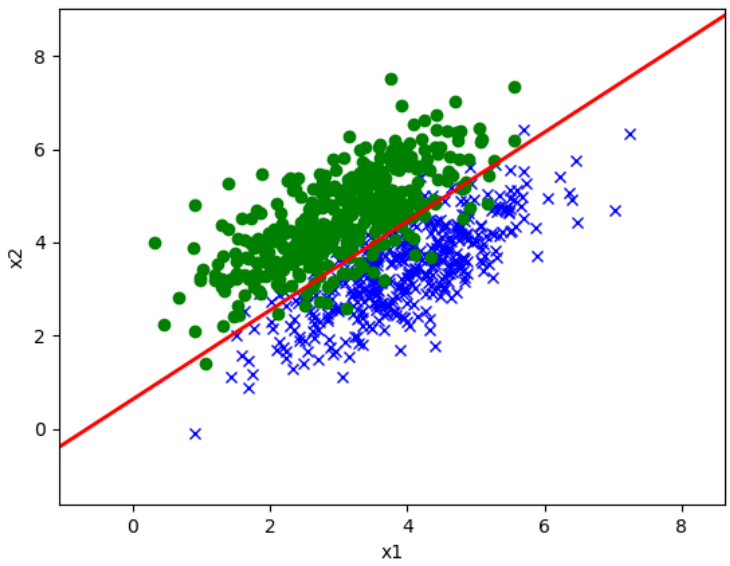


GDA

(g)



logistic regression



GDA

On Dataset 1 GDA perform worse than logistic regression.

Because $p(x|y)$ may be not Gaussian distribution.

(h) Box-Cox transformation的具体解释在PS1-1 Linear Classifiers.ipynb里

Box-Cox transformation.

2.

(a)

$$P(y=1|t=1,x)P(t=1|x)P(x) = P(y=1,t=1,x) = P(t=1|y=1,x)P(y=1|x)P(x)$$

$$P(t=1|x) = P(y=1|x)\frac{P(t=1|y=1,x)}{P(y=1|t=1,x)}$$

$$P(t=1|y=1,x) = 1,\ P(y=1|t=1,x) = P(y=1|t=1)$$

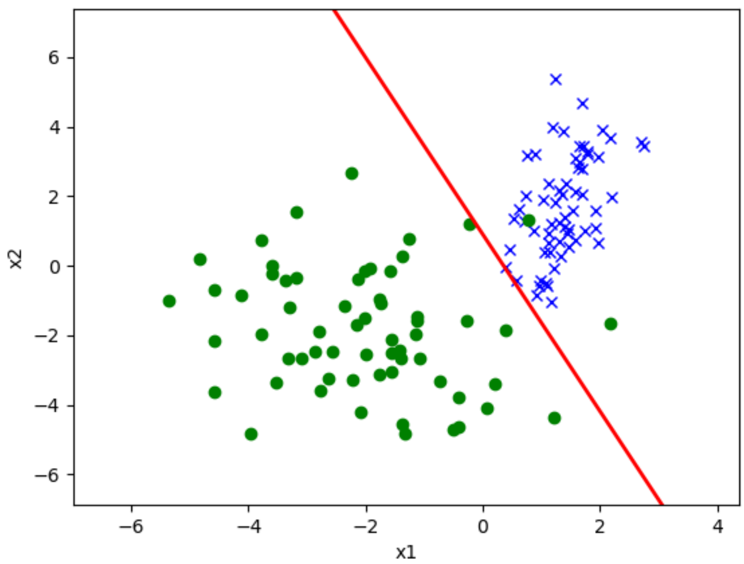
$$P(t=1|x) = \frac{P(y=1|x)}{P(y=1|t=1)}$$

$$P(y=1|t=1) = \alpha$$

(b)

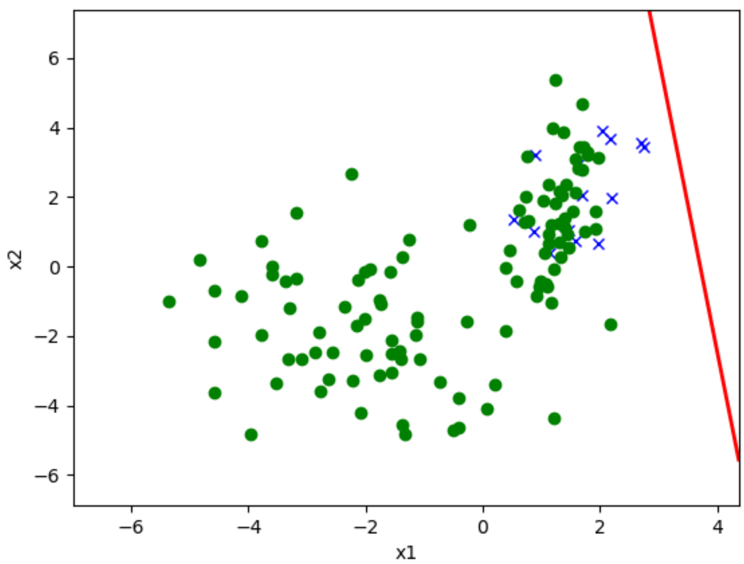
$$h(x) \approx p(y=1|x) = p(t=1|x)\alpha \approx \alpha \quad \text{for all } x \in V_+$$

(c)



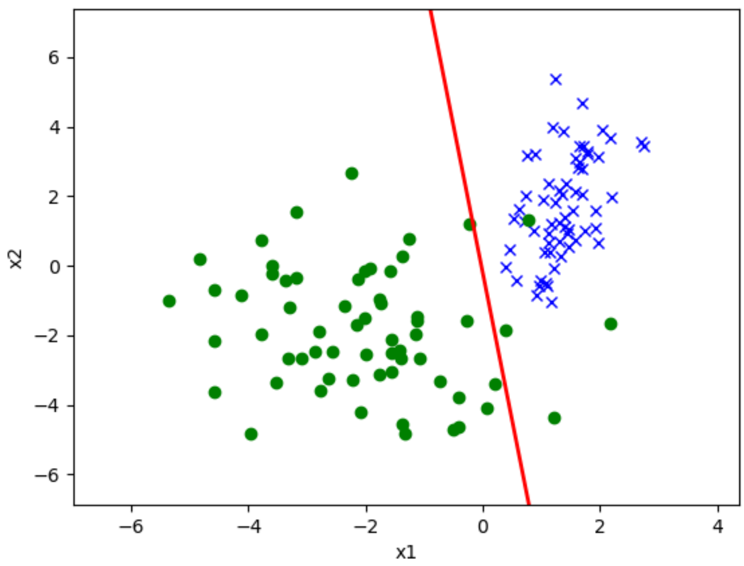
train use t-label

(d)



train use y-label

(e)



train use y-label, rescale by α

3.

(a)

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

$$\begin{cases} b(y) &= \frac{1}{y!} \\ \eta &= \log\lambda \\ T(y) &= y \\ a(\eta) &= e^{\eta} \end{cases}$$

(b)

$$h_\theta(x) = E(y|x;\theta) = \lambda = e^{\eta} = e^{\theta^T x}$$

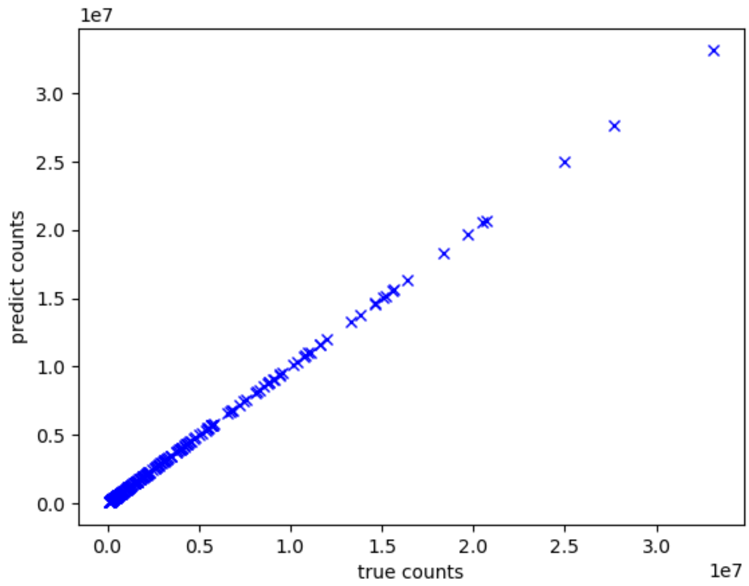
(c)

$$\begin{aligned} \log p(y^{(i)}|x^{(i)};\theta) &= \log\frac{1}{y^{(i)}!}\exp\{\theta^T x^{(i)} y^{(i)} - e^{\theta^T x^{(i)}}\} \\ &= -\log y^{(i)}! + \theta^T x^{(i)} y^{(i)} - e^{\theta^T x^{(i)}} \end{aligned}$$

$$\frac{\partial \log p(y^{(i)}|x^{(i)};\theta)}{\partial\theta_j} = y^{(i)} x_j^{(i)} - e^{\theta^T x^{(i)}} \cdot x_j^{(i)} = (y^{(i)} - e^{\theta^T x^{(i)}}) x_j^{(i)}$$

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

(d)



4.

(a)

$$\frac{\partial}{\partial \eta}\int p(y;\eta)dy = 0$$

$$\begin{aligned}
\frac{\partial}{\partial \eta}\int p(y;\eta)dy &= \int \frac{\partial}{\partial \eta} p(y;\eta)dy \\
&= \int b(y)\exp\{\eta y - a(\eta)\}(y - \frac{\partial a(\eta)}{\partial \eta})dy \\
&= \int p(y;\eta)(y - \frac{\partial a(\eta)}{\partial \eta})dy \\
&= \int yp(y;\eta)dy - \frac{\partial a(\eta)}{\partial \eta}\int p(y;\eta)dy \\
&= E[Y;\eta] - \frac{\partial a(\eta)}{\partial \eta}
\end{aligned}$$

$$E[Y;\eta] = E[Y|X;\theta] = \frac{\partial a(\eta)}{\partial \eta}$$

(b)

$$\frac{\partial}{\partial \eta}\int yp(y;\eta)dy = \frac{\partial^2 a(\eta)}{\partial \eta^2}$$

$$\begin{aligned}
\frac{\partial}{\partial \eta}\int yp(y;\eta)dy &= \int y\frac{\partial}{\partial \eta} p(y;\eta)dy \\
&= \int yp(y;\eta)(y - \frac{\partial a(\eta)}{\partial \eta})dy \\
&= \int y^2 p(y;\eta)dy - \frac{\partial a(\eta)}{\partial \eta}\int yp(y;\eta)dy \\
&= E[Y^2;\eta] - E^2[Y;\eta] \\
&= Var[Y;\eta]
\end{aligned}$$

$$Var[Y;\eta] = Var[Y|X;\theta] = \frac{\partial^2 a(\eta)}{\partial \eta^2}$$

(c)

$$
\begin{aligned}
\ell(\theta) &= -\sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)};\theta) \\
&= \sum_{i=1}^{m} -\log b(y^{(i)}) - \theta^T x^{(i)} y^{(i)} + a(\theta^T x^{(i)})
\end{aligned}
$$

$$
\frac{\partial \ell(\theta)}{\partial \theta_j} = \sum_{i=1}^{m} [a'(\theta^T x^{(i)}) - y^{(i)}] x_j^{(i)}
$$

$$
H_{jk} = \frac{\partial^2 \ell(\theta)}{\partial \theta_j \theta_k} = \sum_{i=1}^{m} a''(\theta^T x^{(i)}) x_j^{(i)} x_k^{(i)}
$$

$$
\begin{aligned}
z^T H z &= \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{n} a''(\theta^T x^{(i)}) x_j^{(i)} x_k^{(i)} z_j z_k \\
&= \sum_{i=1}^{m} a''(\theta^T x^{(i)}) [(x^{(i)})^T z]^2
\end{aligned}
$$

$$
a''(\theta^T x) = Var[Y|X;\theta] \geq 0 \ \Rightarrow \ z^T H z \geq 0
$$

5.

(a)

i.

$$
W \in \mathbb{R}^{m \times m}
$$

$$
W_{ij} = \begin{cases} \frac{1}{2} w^{(i)} & i = j \\ 0 & i \neq j \end{cases}
$$

ii.

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta (X\theta - y)^T W (X\theta - y) \\
&= \nabla_\theta (\theta^T X^T - y^T) W (X\theta - y) \\
&= \nabla_\theta (\theta^T X^T W X \theta - y^T W X \theta - \theta^T X^T W y + y^T W y) \\
&= \nabla_\theta (\theta^T X^T W X \theta - 2 y^T W X \theta) \\
&= 2 X^T W X \theta - 2 X^T W y
\end{aligned}
$$

$$
\nabla_\theta J(\theta) = 0 \ \Rightarrow \ \theta = (X^T W X)^{-1} X^T W y
$$

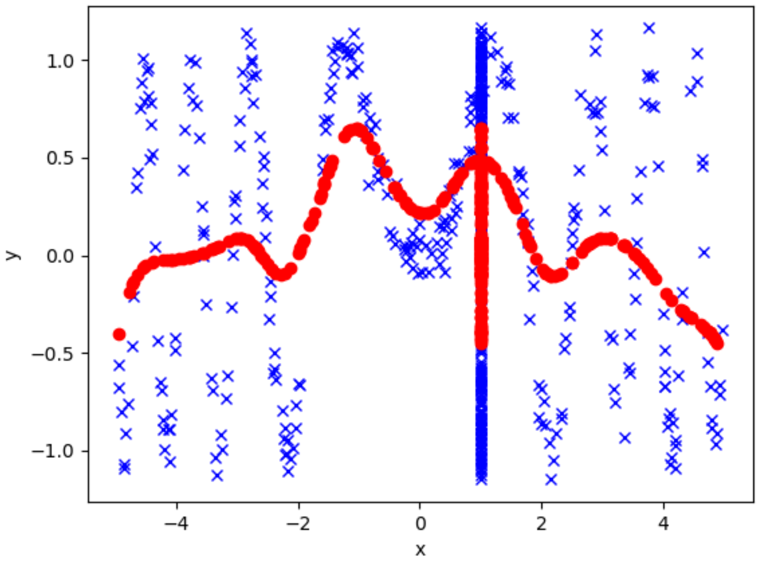
iii.

$$
\begin{aligned}
\ell(\theta) &= \sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)};\theta) \\
&= \sum_{i=1}^{m} -\log(\sqrt{2\pi}\sigma^{(i)}) - \frac{(y^{(i)} - \theta^T x^{(i)})^2}{2(\sigma^{(i)})^2}
\end{aligned}
$$

$$
w^{(i)} = -\frac{1}{(\sigma^{(i)})^2}
$$

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

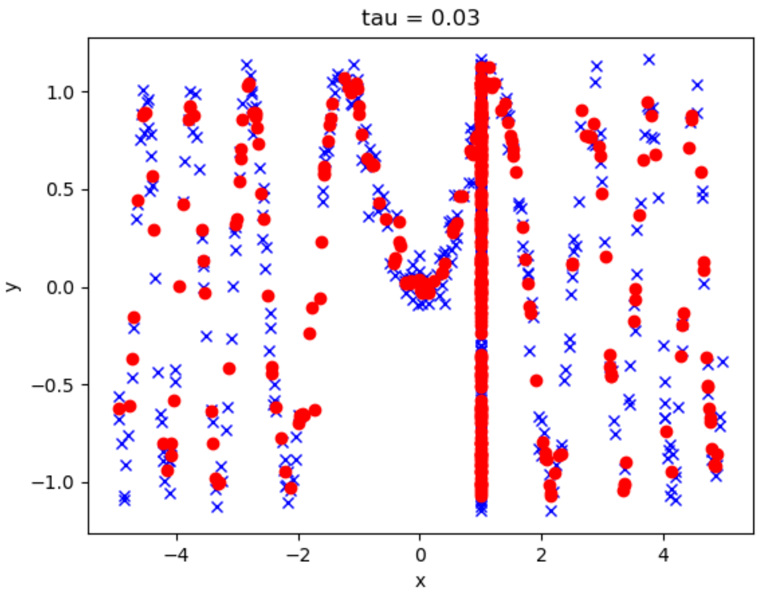
(b)

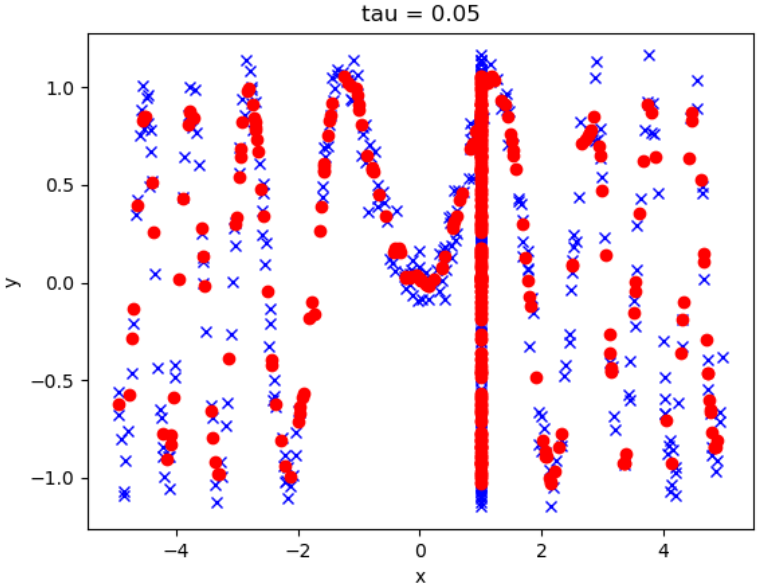


MSE=0.331.

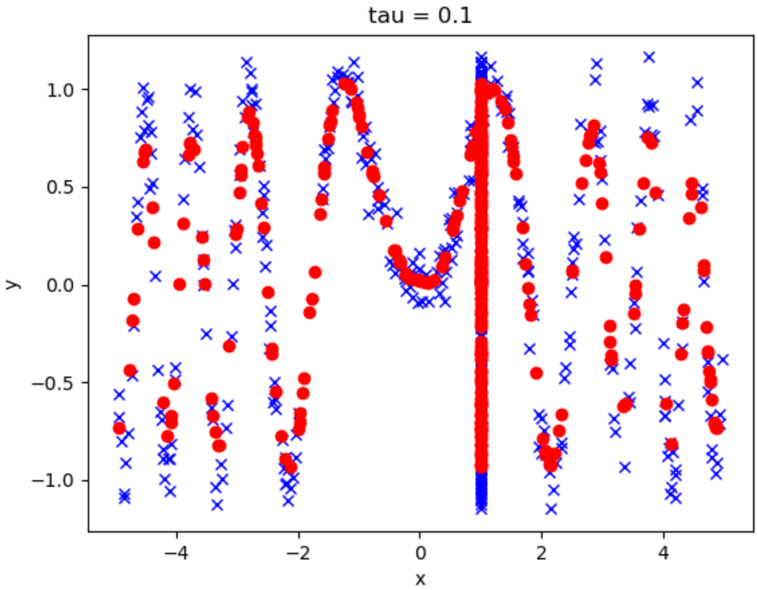
The model seems to be underfitting.

(c)

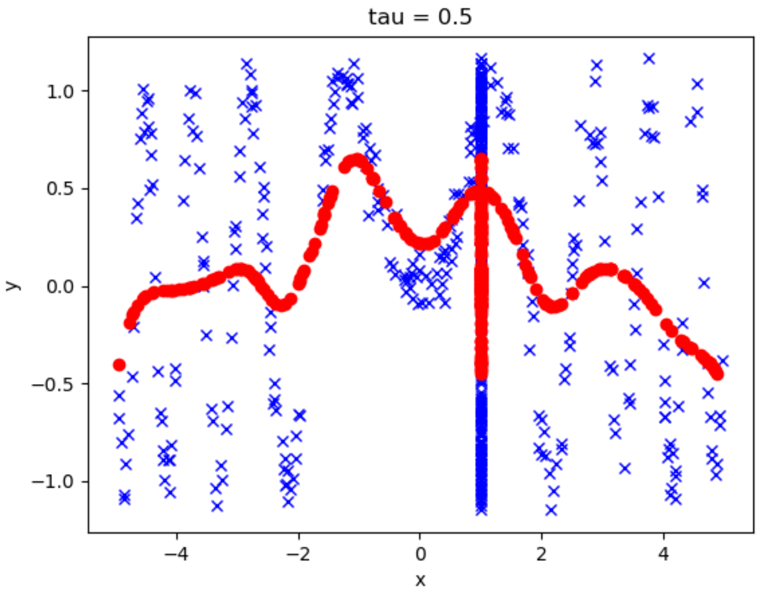




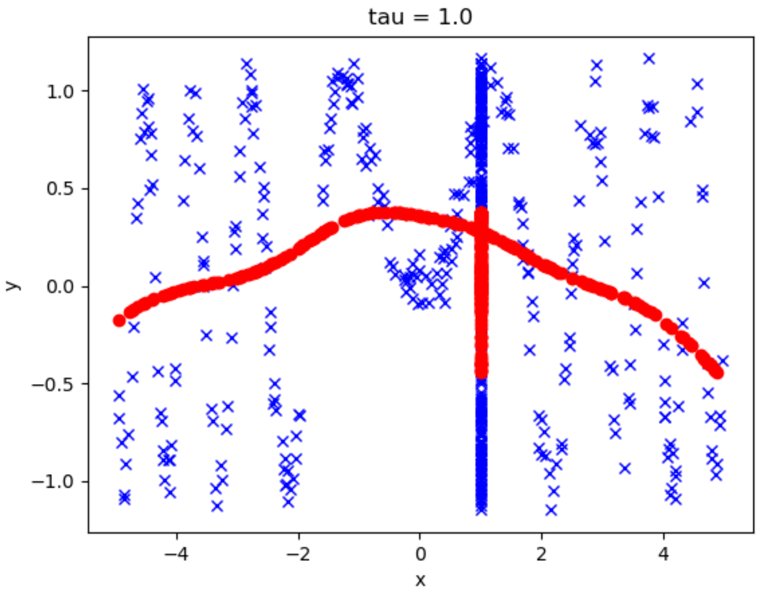
tau = 0.05
1.0
0.5
0.0
−0.5
−1.0
y
−4
−2
0
2
4
x

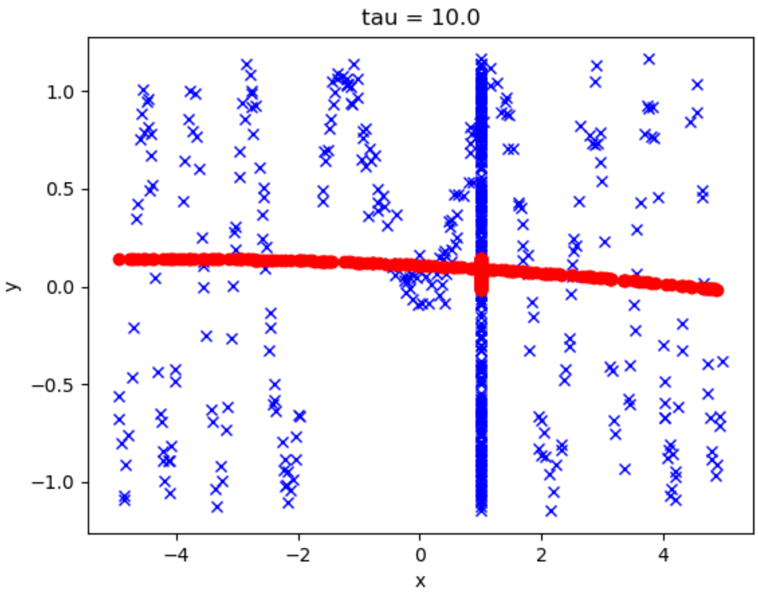


tau = 0.1
1.0
0.5
0.0
−0.5
−1.0
y
−4
−2
0
2
4
x



tau = 0.5
1.0
0.5
0.0
−0.5
−1.0
y
−4
−2
0
2
4
x





$\tau = 0.05$ achieves the lowest MSE on the valid set.

MSE=0.012 on the valid set, MSE=0.017 on the test set.