CS 229, Fall 2017 Problem Set #1: Supervised Learning

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19-10-2017

Disclaimer

These problem sets have been developed by the CS229 team at Stanford University. If you are following this course or a related one, please consider whether checking my solutions might constitute a violation of the honour code.

1 Logistic regression

a. Consider the average empirical loss (the risk) for logistic regression:

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

where $y^{(i)} \in \{-1, 1\}$, $h_\theta = g(\theta^T x)$ and $g(z) = 1/(1 + e^{-x})$. Find the Hessian H of this function, and show that for any vector z_1 holds true that

$$z_1^T H z_1 \geq 0$$

Solution

Hessian:

$$\frac{\delta J}{\delta \theta_j} = \frac{1}{m}\sum_{i=1}^{m} \left[\left(\frac{1}{1 + e^{-y^{(i)}\theta^T x^{(i)}}} \right) \left(e^{-y^{(i)}\theta^T x^{(i)}} \right) \left(-y^{(i)} x_j^{(i)} \right) \right]$$

$$
\begin{aligned}
H_{jk} &= \frac{\delta J}{\delta \theta_j \theta_k} \\
&= \frac{1}{m} \sum_{i=1}^{m} \left[\left(\frac{-1}{\left(1 + e^{-y^{(i)}\theta^T x^{(i)}}\right)^2} \right) \left(e^{-y^{(i)}\theta^T x^{(i)}} \right) \left(-y^{(i)} x_k^{(i)} \right) \left(e^{-y^{(i)}\theta^T x^{(i)}} \right) \left(-y^{(i)} x_j^{(i)} \right) \right. \\
&+ \left. \left(\frac{1}{1 + e^{-y^{(i)}\theta^T x^{(i)}}} \right) \left(e^{-y^{(i)}\theta^T x^{(i)}} \right) \left(-y^{(i)} x_k^{(i)} \right) \left(e^{-y^{(i)}\theta^T x^{(i)}} \right) \left(-y^{(i)} x_j^{(i)} \right) \right] \\
&= \frac{1}{m} \sum_{i=1}^{m} \left[\underbrace{\frac{e^{-y^{(i)}\theta^T x^{(i)}}}{1 + e^{-y^{(i)}\theta^T x^{(i)}}}}_{\in (0,1)} \left(y^{(i)} \right)^2 x_j^{(i)} x_k^{(i)} \left(1 - \underbrace{\frac{e^{-y^{(i)}\theta^T x^{(i)}}}{1 + e^{-y^{(i)}\theta^T x^{(i)}}}}_{\in (0,1)} \right) \right] \\
&= \frac{1}{m} \sum_{i=1}^{m} \left[C_i x_j^{(i)} x_k^{(i)} \right] \text{ where } C_i \geq 0
\end{aligned}
$$

$$
\begin{aligned}
z_{1j}^T H_{jk} z_{1k} &= \sum_{j=1}^{n+1} z_j \left(\sum_{k=1}^{n+1} \left(\sum_{i=1}^{m} \left[\frac{C_i}{m} x_j^{(i)} x_k^{(i)} \right] z_k \right) \right) \\
&= \sum_{i=1}^{m} \frac{C_i}{m} \left(\sum_{j=1}^{n+1} \sum_{k=1}^{n+1} z_j x_j^{(i)} x_k^{(i)} z_k \right) = \sum_{i=1}^{m} \frac{C_i}{m} \left({x^{(i)}}^T z \right)^2 \geq 0
\end{aligned}
$$

b. We have provided two data files:

- `http://cs229.stanford.edu/ps/ps1/logistic_x.txt`
- `http://cs229.stanford.edu/ps/ps1/logistic_y.txt`

These files contain the inputs ($x^{(i)} \in \mathbb{R}^2$) and outputs ($y^{(i)} \in \{-1, 1\}$), respectively for a binary classification problem, with one training example per row. Implement Newton's method for optimizing $J(\theta)$, and apply it to fit a logistic regression model to the data. Initialize Newton's method with $\theta = \vec{0}$ (the vector of all zeros). What are the coefficients θ resulting from your fit?

Solution

$\theta = [-2.62, \quad 0.76, \quad 1.17]$

See scripts folder for the full code.

c. Plot the training data (your axes should be x_1 and x_2, corresponding to the two coordinates of the inputs, and you should use a different symbol for each point plotted to indicate whether that example had label 1 or -1). Also plot on the same figure the decision boundary fit by logistic regression. (This should be a straight line showing the boundary separating the region where $h_\theta(x) > 0.5$ from where $h_\theta(x) \leq 0.5$.)

Solution

The boundary line is defined by $h_\theta = 0.5$. Since h_θ is the logistic regression, that is equivalent to enforce $\theta^T x = 0$.

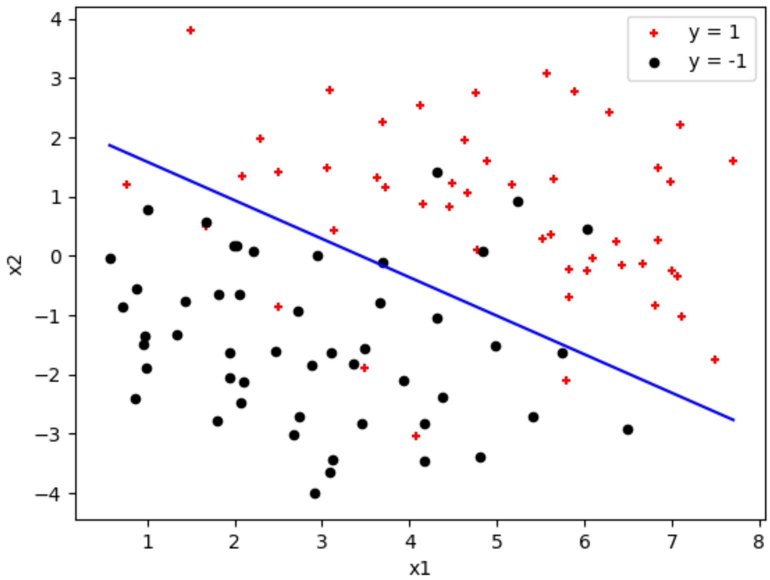


Figure 1: Training set and hypothesis $h_\theta(x) = 0.5$

2 Poisson regression and the exponential family

a. Consider the Poisson distribution parameterized by λ:

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

Show that the Poisson distribution is in the exponential family, and clearly state what are $b(y)$, η, $T(y)$, and $a(\eta)$.

Solution

For the generic exponential family,

$$p(y; \eta) = b(y)\exp(\eta^T T(y) - a(\eta)) \tag{1}$$
$$\log p(y; \eta) = \log(b(y)) + \eta^T T(y) - a(\eta) \tag{2}$$

For the Poisson distribution,

$$p(y; \lambda) = \frac{e^{-\lambda}\lambda^y}{y!} \tag{3}$$
$$\log p(y; \lambda) = \log \frac{1}{y!} + y \log \lambda - \lambda \tag{4}$$

And so from (2) and (4), the Poisson distribution is part of the exponential family, where:

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

b. Consider performing regression using a GLM model with a Poisson response variable. What is the canonical response function for the family? (You may use the fact that a Poisson random variable with parameter λ has mean λ.)

Solution

Canonical response function $= E[T(y);\eta] = E[y;\eta(\lambda)] \overset{y\sim Poisson}{=} \lambda = \exp(\eta)$.

c. For a training set $\{(x^{(i)}, y^{(i)}); i = 1, ..., m\}$, let the log-likelihood of an example be $\log p(y^{(i)}|x^{(i)};\theta)$. By taking the derivative of the log-likelihood with respect to θ_j , derive the stochastic gradient ascent rule for learning using a GLM model with Poisson responses y and the canonical response function.

Solution

As a precondition for applying GLM, $\eta^{(i)} = \theta^T x^{(i)}$.

$$\begin{aligned} l^{(i)}(\theta) = \log p^i &\overset{(4)}{=} \log \frac{1}{y^{(i)}!} + y^{(i)}\eta^i - \exp(\eta^i) \\ &= \log \frac{1}{y^{(i)}!} + y^{(i)}\theta^T x^{(i)} - \exp(\theta^T x^{(i)}) \\ l(\theta) &= \sum_{i=1}^{m} l^{(i)}(\theta) \end{aligned}$$

Since we are asked for stochastic gradient descent, we will only consider the gradient $\frac{\delta l^{(i)}(\theta)}{\delta \theta_j}$.

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

Stochastic gradient ascent rule:

Loop until convergence {

for $i = 1, ..., m$ {

$\theta_j = \theta_j + \alpha \frac{\delta l^{(i)}(\theta)}{\delta \theta_j} \quad \forall j$

}

}

d. Consider using GLM with a response variable from any member of the exponential family in which $T(y) = y$, and the canonical response function $h(x)$ for the family. Show that stochastic gradient ascent on the log-likelihood log $p(y|X;\theta)$ results in the update rule $\theta_i := \theta_i - \alpha(h(x) - y)x_i$.

Solution

What needs to be proved is that $\frac{\delta \log p^i}{\delta \theta_j} = (y^{(i)} - h(x^{(i)}))x_j^{(i)} \quad \forall i$. From the definition of a GLM (see (2)),

$$\begin{aligned}
\log p^i &= \log(b(y^{(i)}) + {\eta^i}^T T(y^{(i)}) - a(\eta^i) \\
&= \log(b(y^{(i)})) + (\theta^T x^{(i)})^T y^{(i)} - a(\theta^T x^{(i)}) \\
\frac{\delta \log p^i}{\delta \theta_j} &= y^{(i)} x_j^{(i)} - \frac{\delta a(\eta^i)}{\delta(\eta^i)} x_j^{(i)}
\end{aligned}$$

And so what we finally should prove is that $h(\theta^T x^{(i)}) = h(\eta^i) = \frac{\delta a(\eta^i)}{\delta(\eta^i)}$.

By the definition of a probability distribution,

$$\begin{aligned}
1 &= \int_{-\infty}^{+\infty} b(y^{(i)}) \exp({\eta^i}^T y^{(i)}) \exp(-a(\eta^i)) \mathrm{d}y \quad \forall i \\
\exp(-a(\eta^i)) &= \frac{1}{\int_{-\infty}^{+\infty} b(y^{(i)}) \exp({\eta^i}^T y^{(i)}) \mathrm{d}y} \\
\frac{\delta \exp(-a(\eta^i))}{\delta \eta^i} &= \frac{-\int_{-\infty}^{+\infty} b(y^{(i)}) y^{(i)} \exp\left({\eta^i}^T \left(y^{(i)} - 1\right)\right) \exp\left(\eta^i\right) \mathrm{d}y}{\left(\int_{-\infty}^{+\infty} b(y^{(i)}) \exp({\eta^i}^T y^{(i)}) \mathrm{d}y\right)^2} \\
-\frac{\delta a}{\delta \eta^i} \exp(-a(\eta^i)) &= -\exp(a(\eta^i))^2 \int_{-\infty}^{+\infty} y \cdot p(y|x) \mathrm{d}y \\
&= -\exp(a(\eta^i)) E[y^{(i)}; \eta^i] = -\exp(a(\eta^i)) h(\eta^i)
\end{aligned}$$

And by simplifying on both sides of the equality,

$$\frac{\delta a(\eta^i)}{\delta(\eta^i)} = h(\eta^i)$$

3 Gaussian discriminant analysis

Suppose we are given a dataset $\{(x^{(i)}, y^{(i)}); i = 1, ..., m\}$ consisting of m independent examples, where $x^{(i)} \in \mathbb{R}^n$ are n-dimensional vectors, and $y^{(i)} \in \{-1, 1\}$. We will model the joint distribution of (x, y) according to:

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

Here, the parameters of our model are ϕ, Σ, μ_1 and μ_{-1}.

a. Suppose we have already fit ϕ, Σ, μ_1 and μ_{-1}, and now want to make a prediction at some new query point x. Show that the posterior distribution of the label at x takes the form of a logistic function, and can be written

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

where $\theta \in \mathbb{R}^n$ and the bias term $\theta_0 \in (R)$ are some appropriate functions of ϕ, Σ, μ_1 and μ_{-1}.

<u>Solution</u>

For easiness in the development, let A and E_i be

$$
\begin{aligned}
A &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \\
E_i &= \exp\left(-\frac{1}{2}(x-\mu_i)^T\Sigma^{-1}(x-\mu_i)\right) \quad \text{with} \quad i \in \{-1, 1\}
\end{aligned}
$$

$$
\begin{aligned}
p(y|x;params) &= \frac{p(x|y)p(y)}{p(x)} \\
p(x) = p(x|y=1)&p(y=1) + p(x|y=-1)p(y=-1)
\end{aligned}
$$

Therefore,

$$
p(y|x;params) = \begin{cases} \dfrac{E_1\phi}{E_1\phi + E_{-1}(1-\phi)} & y = 1 \\ \dfrac{E_{-1}(1-\phi)}{E_1\phi + E_{-1}(1-\phi)} & y = -1 \end{cases}
$$

Expressing $p(y|x;params)$ in a compact way,

$$
\begin{aligned}
p(y|x) &= \frac{1}{1+B(x)^{-y}} \quad \text{where} \\
B(x) &= \frac{E_1\phi}{E_{-1}(1-\phi)}
\end{aligned}
$$

We can now elaborate on $B(x)$:

$$B(x) = \exp\left(\underbrace{-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) + \frac{1}{2}(x-\mu_{-1})^T\Sigma^{-1}(x-\mu_{-1})}_{C(x)}\right)$$
$$\cdot \exp\left(\underbrace{\log\left(\frac{\phi}{1-\phi}\right)}_{D}\right)$$

$C(x)$ seems like a quadratic function of x, but the second order terms cancel out, and what is left is an affine function of x of the type $C(x) = C_1 x + X_0$.

Renaming, $\exp(C_1 x + C_0 + D) = \exp(\theta_1 x + \theta_0)$, and hence:

$$p(y|x) = \frac{1}{1 + \exp(\theta_1 x + \theta_0)^{-y}}$$

b. For this part of the problem only, you may assume n (the dimension of x) is 1, so that $\Sigma = [\sigma^2]$ is just a real number, and likewise the determinant of Σ is given by $|\Sigma| = \sigma^2$. The log-likelihood of the data is

$$\begin{aligned} l(\phi, \Sigma, \mu_1, \mu_{-1}) &= \log \prod_{i=1}^{m} p(x^{(i)}, y^{(i)}; \phi, \Sigma, \mu_1, \mu_{-1}) \\ &= \sum_{i=1}^{m} \log p(x^{(i)}|y^{(i)}; \Sigma, \mu_1, \mu_{-1}) + \sum_{i=1}^{m} \log p(y^{(i)}; \phi) \end{aligned}$$

By maximising l with respect to the parameters, prove that the maximum likelihood estimates of ϕ, Σ, μ_1 and μ_{-1} are indeed as given in the formulas.

Conditional Gaussian distribution: $p(x|y=k) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma^2}\right)$ with $k = \{-1, 1\}$

Prior Bernoulli distribution: $p(y) = \begin{cases} \phi & y = 1 \\ 1-\phi & y = -1 \end{cases}$

Derivatives:

(a) Derivative w.r.t. ϕ:

$$
\begin{aligned}
\frac{\delta l}{\delta \phi} &= \sum_{y^{(i)}=1} \frac{1}{\phi} \cdot 1 + \sum_{y^{(i)}=-1} \frac{1}{(1-\phi)} \cdot (-1) \\
&= \frac{1}{\phi} \sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=1\right\} - \frac{1}{1-\phi} \sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=-1\right\} = 0 \\
\implies (1-\phi) &\sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=-1\right\} - \phi \sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=1\right\} = 0 \\
\implies &- m\phi + \sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=1\right\} = 0 \\
\implies \phi &= \frac{\sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=1\right\}}{m}
\end{aligned}
$$

(b) Derivative w.r.t. μ_{-1}:

$$
\begin{aligned}
\frac{\delta l}{\delta \mu_{-1}} &= \sum_{y^{(i)}=-1} \frac{1}{\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x^{(i)}-\mu_{-1})^2\right)} \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x^{(i)}-\mu_{-1})^2}{2\sigma^2}\right) \frac{(x^{(i)}-\mu_{-1})}{\sigma^2} = 0 \\
\implies &\frac{1}{\sigma^2}\left(\sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=-1\right\} x^{(i)} - \mu_{-1} \sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=-1\right\}\right) = 0 \\
\implies \mu_{-1} &= \frac{\sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=-1\right\} x^{(i)}}{\sum_{i=1}^{m} \mathbb{1}\left\{y^{(i)}=-1\right\}}
\end{aligned}
$$

(c) Derivative w.r.t. μ_1:
Proceeding in the same way as for μ_{-1},

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

(d) Derivative w.r.t. σ^2:

$$\frac{\delta l}{\delta \sigma^2} = \sum_{y^{(i)}=-1}\left[\frac{1}{\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{1}{2\sigma^2}(x^{(i)}-\mu_{-1})^2\right)}\cdot\left(\frac{\pi}{\left(\sqrt{2\pi\sigma^2}\right)^3}\cdot\exp\left(-\frac{(x^{(i)}-\mu_{-1})^2}{2\sigma^2}\right)+\right.\right.$$

$$\left.\left.+\frac{1}{\sqrt{2\pi\sigma^2}}\cdot\frac{+(x^{(i)}-\mu_{-1})^2}{2(\sigma^2)^2}\exp\left(-\frac{(x^{(i)}-\mu_{-1})^2}{2\sigma^2}\right)\right)\right]+$$

$$\sum_{y^{(i)}=1}\left[\frac{1}{\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{1}{2\sigma^2}(x^{(i)}-\mu_{1})^2\right)}\cdot\left(\frac{\pi}{\left(\sqrt{2\pi\sigma^2}\right)^3}\cdot\exp\left(-\frac{(x^{(i)}-\mu_{1})^2}{2\sigma^2}\right)+\right.\right.$$

$$\left.\left.+\frac{1}{\sqrt{2\pi\sigma^2}}\cdot\frac{+(x^{(i)}-\mu_{1})^2}{2(\sigma^2)^2}\exp\left(-\frac{(x^{(i)}-\mu_{1})^2}{2\sigma^2}\right)\right)\right]$$

$$= \sum_{y^{(i)}=-1}\left[\frac{\pi}{2\pi\sigma^2}+\frac{(x^{(i)}-\mu_{-1})^2}{2(\sigma^2)^2}\right]+\sum_{y^{(i)}=1}\left[\frac{\pi}{2\pi\sigma^2}+\frac{(x^{(i)}-\mu_{1})^2}{2(\sigma^2)^2}\right]$$

$$= \frac{m}{2\sigma^2}+\frac{1}{2(\sigma^2)^2}\sum_{i=1}^{m}(x^{(i)}-\mu_{y^{(i)}})^2 = 0$$

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

4 Linear invariance of optimisation algorithms

Consider using an iterative optimization algorithm (such as Newton's method, or gradient descent) to minimize some continuously differentiable function $f(x)$. Suppose we initialize the algorithm at $x^{(0)} = 0$. When the algorithm is run, it will produce a value of $x \in \mathbb{R}^n$ for each iteration: $x^{(1)}, x^{(2)}, ...$

Now, let some non-singular square matrix $A \in \mathbb{R}^{nxn}$ be given, and define a new function $g(z) = f(A \cdot z)$. Consider using the same iterative optimization algorithm to optimize g (with initialization $z^{(0)} = 0$). If the values $z^{(1)}, z^{(2)}, ...$ produced by this method necessarily satisfy $z^{(i)} = A^{-1}x^{(i)} \quad \forall i$, we say this optimization algorithm is invariant to linear reparametrizations.

a. Show that Newton's method (applied to find the minimum of a function) is invariant to linear reparameterizations.

<u>Solution</u>

Newton's method: $z^{(i+1)} = z^{(i)} - \left(\nabla_z g(z^{(i)})\right)^{-1} \cdot g(z^{(i)})$. Multiplying both sides by A,

$$A \cdot z^{(i+1)} = \underbrace{A \cdot z^{(i)}}_{\mathrm{I}} - \underbrace{A \cdot \left(\nabla_z g(z^{(i)})\right)^{-1}}_{\mathrm{III}} \cdot \underbrace{g(z^{(i)})}_{\mathrm{II}}$$

$$\implies x^{(i+1)} = x^{(i)} - \left(\nabla_x f(x^{(i)})\right)^{-1} \cdot f(x^{(i)})$$

where

I. $A \cdot z^{(i)} = x^{(i)}$

II. $g(z^{(i)}) = f(A \cdot z^{(i)}) = f(x^{(i)})$

III. $A \cdot \left(\nabla_z g(z^{(i)})\right)^{-1} = \left(\nabla_z g(z^{(i)}) \cdot A^{-1}\right)^{-1} = \left(\nabla_z f(A \cdot z^{(i)}) \cdot A^{-1}\right)^{-1} = \left(\nabla_{A \cdot z} f(A \cdot z^{(i)})\right)^{-1} = \left(\nabla_x f(x^{(i)})\right)^{-1}$

b. Is gradient descent invariant to linear reparameterizations? Justify your answer.

Solution

Gradient descent: $\theta^{(i+1)} = \theta^{(i)} - \alpha \cdot f(\theta^{(i)})$, where $f(\theta)$ is the function we are trying to minimise. Since α is not a linear function of θ, we cannot establish the equality used in aIII in the previous subsection, and so it is not linearly invariant.

5 Regression for denoising quasar spectra [1]

For the full introduction see the original problem set description located at `http://cs229.stanford.edu/ps/ps1/ps1.pdf`.

Getting the data. We will be using data generated from the Hubble Space Telescope Faint Object Spectrograph (HST-FOS), Spectra of Active Galactic Nuclei and Quasars[2]. We have provided two comma-separated data files located at:

- Training set: `http://cs229.stanford.edu/ps/ps1/quasar_train.csv`
- Test set: `http://cs229.stanford.edu/ps/ps1/quasar_test.csv`

Each file contains a single header row containing 450 numbers corresponding integral wavelengths in the interval [1150, 1600] Å. The remaining lines contain relative flux measurements for each wavelength. Specifically, `quasar_train.csv` contains 200 examples and `quasar_test.csv` contains 50 examples.

a. Locally weighted linear regression

Consider a linear regression problem in which we want to "weight" different training examples differently. Specifically, suppose we want to minimize

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

i Show that $J(\theta)$ can also be written as

$$J(\theta) = (X\theta - y)^T W (X\theta - y)$$

for an appropriate diagonal matrix W. State clearly what W is.

Solution

[1] Ciollaro, Mattia, et al. "Functional regression for quasar spectra." arXiv:1404.3168 (2014)

[2] `https://hea-www.harvard.edu/FOSAGN/`

$$
\begin{aligned}
J(\theta) &= (X\theta - y)^T W (X\theta - y) \\
&= \begin{bmatrix} (X\theta - y)_1 & (X\theta - y)_2 & \cdots & (X\theta - y)_m \end{bmatrix} \begin{bmatrix} W_1 & 0 & \cdots & 0 \\ 0 & W_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & W_m \end{bmatrix} \begin{bmatrix} (X\theta - y)_1 \\ (X\theta - y)_2 \\ \vdots \\ (X\theta - y)_m \end{bmatrix} \\
&= \begin{bmatrix} (X\theta - y)_1 & (X\theta - y)_2 & \cdots & (X\theta - y)_m \end{bmatrix} \begin{bmatrix} W_1(X\theta - y)_1 \\ W_2(X\theta - y)_2 \\ \vdots \\ W_m(X\theta - y)_m \end{bmatrix} \\
&= \sum_{i=1}^{m} W_i (X\theta - y)_i^2
\end{aligned}
$$

where $(X\theta - y)_i = \theta_1 x_1^{(i)} + \ldots + \theta_n x_n^{(i)} - y^{(i)} = \theta^T x^{(i)} - y^{(i)}$ and $W_i = \frac{1}{2} w^{(i)}$.

ii By finding the derivative $\nabla_\theta J(\theta)$ and setting that to zero, generalize the normal equation to this weighted setting, and give the new value of θ that minimizes $J(\theta)$ in closed form as a function for X, W and y.

Solution

$$
\begin{aligned}
\nabla_\theta J(\theta) =& \nabla_\theta \left((X\theta - y)^T W (X\theta - y) \right) = \nabla_\theta \left((\theta^T X^T - y^T)(WX\theta - Wy) \right) \\
=& \nabla_\theta \left(\theta^T X W X \theta - \theta^T X^T W y - y^T W X \theta + y^T W y \right) \\
=& \underbrace{\nabla_\theta tr\left(\theta^T X W X \theta\right)}_{I} - \underbrace{\nabla_\theta tr\left(\theta^T X^T W y\right)}_{II} - \underbrace{\nabla_\theta tr\left(y^T W X \theta\right)}_{III} + \underbrace{\nabla_\theta tr\left(y^T W y\right)}_{=0 \text{ (constant w.r.t. } \theta)} \\
=& \underbrace{2X^T W X \theta}_{I} - \underbrace{X^T W y}_{II} - \underbrace{X^T W y}_{III} \\
=& 2 \cdot \left(X^T W X \theta - X^T W y \right)
\end{aligned}
$$

Setting the gradient to zero,

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

iii Suppose we have a training set $\{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$ of m independent examples, but in which the $y^{(i)}$'s were observed with differing variances. Specifically, suppose that

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

i.e. $y^{(i)}$ has mean $\theta^T x^{(i)}$ and variance $(\sigma^{(i)})^2$ where the $\sigma^{(i)}$'s are fixed, known constants. Show that finding the maximum likelihood estimate of θ reduces to solving a weighted linear regression problem. State clearly what the $w^{(i)}$'s are in terms of the $\sigma^{(i)}$'s.

Solution

Maximising the likelihood is equivalent to maximising the log-likelihood $l(\theta)$.

$$l(\theta) = \sum_{i=1}^{m} \log\left(p(y^{(i)}|x^{(i)};\theta)\right) = \sum_{i=1}^{m} \log\left(\frac{1}{\sqrt{2\pi}\sigma^{(i)}}\right) - \sum_{i=1}^{m} \frac{(y^{(i)} - \theta^T x^{(i)})^2}{2(\sigma^{(i)})^2}$$

Since the first term is known and constant, we only need to maximise

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

which is just $J(\theta)$ when $w^{(i)} = \frac{-1}{2\left(\sigma^{(i)}\right)^2}$.

b. Visualising the data

i Use the normal equations to implement (unweighted) linear regression $y = \theta^T X$) on the *first* training example. On one figure, plot both the raw data and the straight line resulting from your fit. State the optimal θ resulting from the linear regression.

Solution

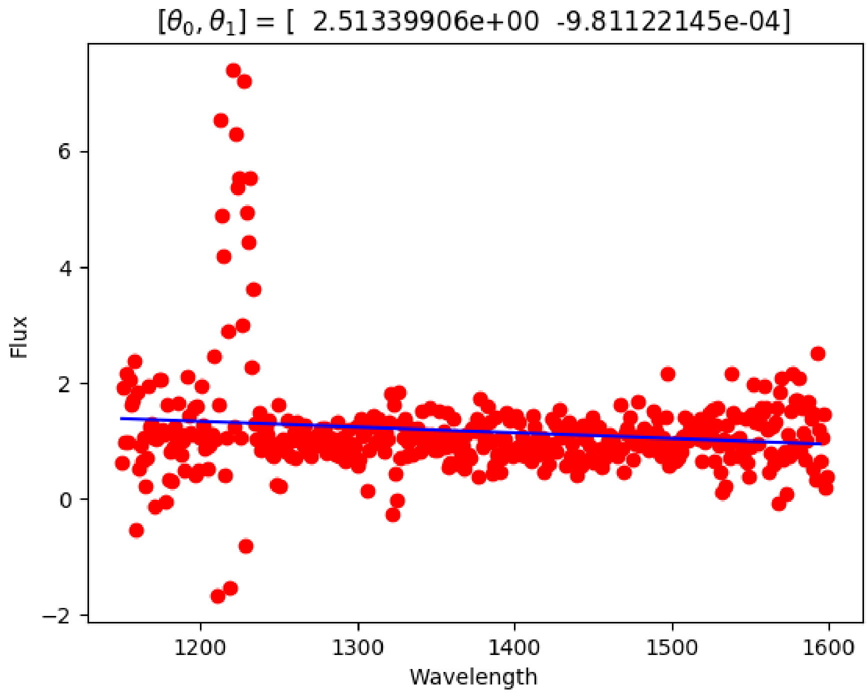


Figure 2: First training example and linear fit

ii Implement locally weighted linear regression on the *first* training example. Use the normal equations derived in part aii. On a different figure, plot both the raw data and the smooth curve resulting from your fit. When evaluating $h(\cdot)$ at a query point x, use weights

$$w^{(i)} = \exp\left(-\frac{(x - x^{(i)})^2}{2\tau^2}\right),$$

with bandwidth parameter $\tau = 5$.
Solution

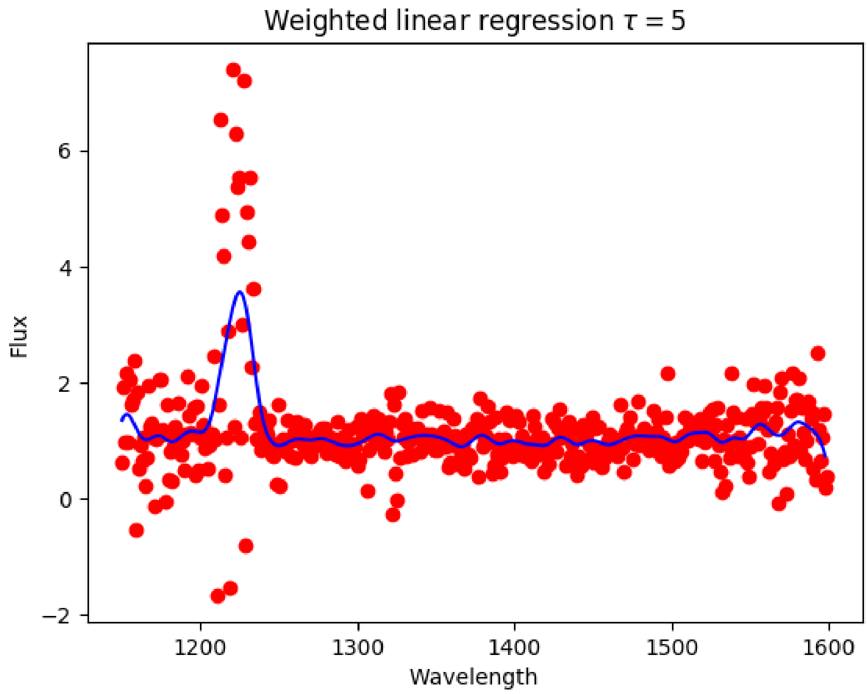
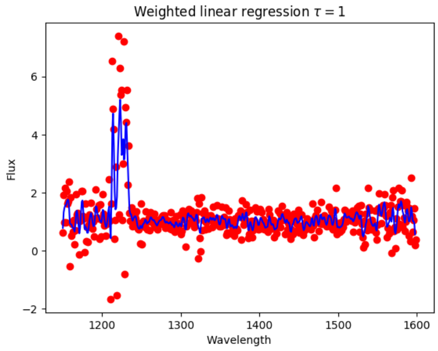
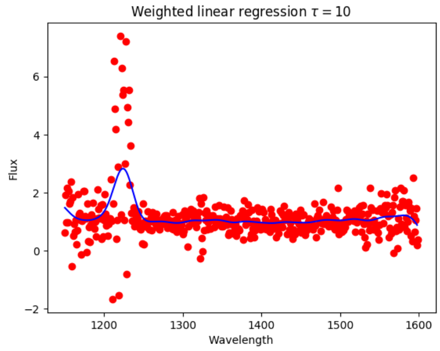


Figure 3: First training example and weighted fit

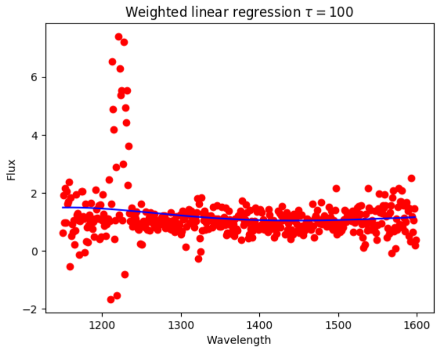
iii Repeat the previous step four more times with $\tau = 1, 10, 100$ and 1000. Plot the resulting curves. Comment on what happens to the locally weighted linear regression line as τ varies.
Solution



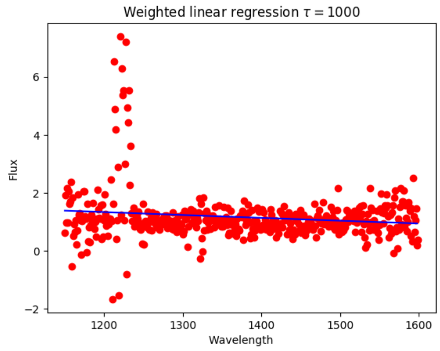
(a) $\tau = 1$



(b) $\tau = 10$



(c) $\tau = 100$



(d) $\tau = 1000$

The larger the bandwidth parameter, the further the examples with a significant weight for a given x. In the limit, when $\tau \to \infty$ the result is a flat distribution of weights, and we retrieve the linear regression model, very underfitted. On the other hand, when $\tau \to 0$ the weight distribution will be very localised, leading to an overfitted model very sensitive to any individual example.