

# CS229 Fall 2017, Problem Set #1: Supervised Learning

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Collaborators:

By turning in this assignment, I agree by the Stanford honor code and declare that all of this is my own work.

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## 1. Logistic regression

Average empirical loss for logistic regression:

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

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

(a)

$$\begin{aligned} \nabla_{\theta} J(\theta) &= -\frac{1}{m} \sum_{i=1}^m \frac{1}{g(\theta^T y^{(i)} x^{(i)})} \nabla_{\theta} g(\theta^T y^{(i)} x^{(i)}) \\ &= -\frac{1}{m} \sum_{i=1}^m \frac{1}{g(\theta^T y^{(i)} x^{(i)})} y^{(i)} x^{(i)} g(\theta^T y^{(i)} x^{(i)}) (1 - g(\theta^T y^{(i)} x^{(i)})) \\ &= -\frac{1}{m} \sum_{i=1}^m \frac{1}{y^{(i)}} x^{(i)} (1 - g(\theta^T y^{(i)} x^{(i)})) \end{aligned}$$

$$\begin{aligned} H_{i,j} &= \frac{\partial}{\partial \theta_j} [\nabla_{\theta} J(\theta)]_i = \frac{1}{m} \sum_{i=1}^m (y^{(i)})^2 x_j^{(i)} x_i^{(i)} g(\theta^T y^{(i)} x^{(i)}) (1 - g(\theta^T y^{(i)} x^{(i)})) \\ &= \frac{\partial}{\partial \theta_j} [\nabla_{\theta} J(\theta)]_i \end{aligned} \quad \text{H is symmetric}$$

Let's show that for any vector  $z$ ,  
 $z^T H z \geq 0$

$$\sum_i \sum_j z_i x_i x_j z_j = \sum_i z_i x_i \sum_j z_j x_j = (x^T z)(x^T z) = (x^T z)^2 \geq 0$$

$$\begin{aligned} z^T H z &= \sum_i z_i^T (H z)_i = \sum_i \sum_j z_i (H_{i,j}) z_j \\ &= \sum_i \sum_j z_i \left( \frac{1}{m} \sum_{k=1}^m (y^{(k)})^2 x_j^{(k)} x_i^{(k)} g(\theta^T y^{(k)} x^{(k)}) (1 - g(\theta^T y^{(k)} x^{(k)})) \right) z_j \\ &= \frac{1}{m} \sum_{k=1}^m \sum_i \sum_j (y^{(k)})^2 z_j x_j^{(k)} z_i x_i^{(k)} g(\theta^T y^{(k)} x^{(k)}) (1 - g(\theta^T y^{(k)} x^{(k)})) \\ &= \frac{1}{m} \sum_{k=1}^m (y^{(k)})^2 g(\theta^T y^{(k)} x^{(k)}) (1 - g(\theta^T y^{(k)} x^{(k)})) ((x^{(k)})^T z)^2 \end{aligned}$$

For any vector  $z$ ,  $g(z) \in [0, 1]$ , hence  $z^T H z \geq 0$ .

This implies that  $H$  is positive semi-definite, therefore  $J$  is convex and has no local minima other than the global one.

- (b) After implementing Newton's method for optimizing  $J(\theta)$  and applying it to fit a logistic regression model to the data, I obtained a parameter vector:  
 $\theta = [-2.61847133, 0.75979248, 1.1707512]^T$ .

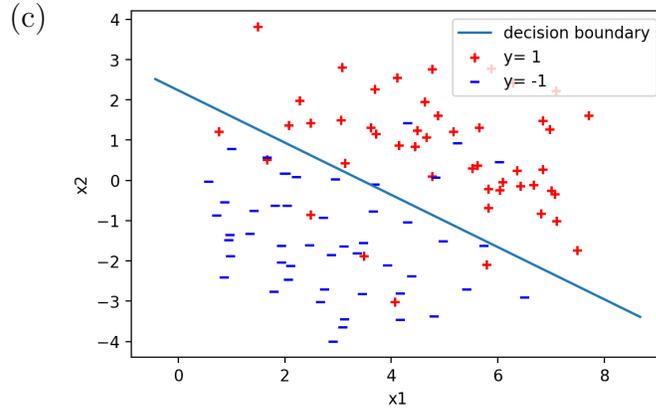


Figure 1: Training data and decision boundary fit by logistic regression

## 2. Poisson regression and the exponential family

(a) We consider the Poisson distribution parametrized by  $\lambda$ :

$$p(y; \lambda) = \frac{e^{-\lambda} \lambda^y}{y!} = \frac{\exp(y \log(\lambda) - \lambda)}{y!} = b(y)(\exp(\eta^T T(y) - a(\eta)))$$

The Poisson distribution is in the exponential family, with:

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

(b) We want to perform regression using a GLM model with a Poisson response variable. To construct the GLM model, we make the following assumptions: -  $y|x; \theta \sim \text{ExponentialFamily}(\eta)$   
- our goal is to predict the expected value of  $T(y)$  given  $x$ . Because  $T(y)=y$ , this means we would like the hypothesis  $h_\theta(x)$  to satisfy:  $h_\theta(x) = \mathbb{E}[y|x]$   
- The natural parameter  $\eta$  and the inputs  $x$  are related linearly  $\eta = \theta^T x$ . It follows that our hypothesis will output:

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

Therefore, the canonical response of this family is  $g(z) = h(\theta^T z) = e^z$ .

(c) Our model assumes that the conditional probability of  $y$  given  $x$  is:

$$p(y^{(i)}|x^{(i)}; \theta) = \frac{\exp(y^{(i)} \theta^T x^{(i)} - e^{\theta^T x^{(i)}})}{y^{(i)}!}$$

We now maximize the likelihood  $L(\theta)$  of our parameter  $\theta$  using gradient ascent.

$$\begin{aligned} \ell(\theta) &= \log(L(\theta)) = \log(p(y^{(i)}|x^{(i)}; \theta)) = y^{(i)} \theta^T x^{(i)} - e^{\theta^T x^{(i)}} - \log(y^{(i)}!) \\ \frac{\partial \ell(\theta)}{\partial \theta_j} &= y^{(i)} x_j^{(i)} e^{-\theta^T x^{(i)}} = x_j^{(i)} (y^{(i)} - e^{\theta^T x^{(i)}}) \end{aligned}$$

We obtain the following stochastic gradient ascent update rule:

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

with  $h_\theta(x) = e^{\theta^T x}$

- (d) We now use GLM for any member of the exponential family for which  $T(y) = y$ , and the canonical response  $h(x)$  for the family. From our model's assumptions,

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

$$\ell(\theta) = \log p(y|X; \theta) = \eta^T y - a(\eta) + \log(b(y))$$

For a single parameter  $\theta_i$ ,

$$\frac{\partial \ell(\theta)}{\partial \theta_i} = \frac{\partial}{\partial \theta_i} (\theta^T x)^T y - \frac{\partial}{\partial \theta_i} a(\theta^T x)$$

To determine  $a(\eta)$ , we use the fact that for  $p(y|X; \theta)$  to be a pdf, it must integrate to 1.

$$\int_y p(y|X; \theta) dy = 1$$

$$\int_y b(y)(\exp(\eta^T T(y) - a(\eta))) dy = 1$$

$$e^{a(\eta)} = \int_y b(y) \exp(\eta^T y) dy$$

$$a(\eta) = \log \int_y b(y) \exp(\eta^T y) dy$$

Let  $f$  be a differentiable function such that  $a(\eta) = \log f(\eta)$ . Using the chain rule,  $\frac{\partial a(\eta)}{\partial \eta} = \frac{\partial \log f(\eta)}{\partial \eta} = \frac{\partial f(\eta)}{\partial \eta} \frac{1}{f(\eta)}$ . Hence,

$$\begin{aligned} \frac{\partial a(\eta)}{\partial \eta} &= \frac{1}{\int_y b(y) \exp(\eta^T y) dy} \int_y b(y) \frac{\partial \exp(\eta^T y)}{\partial \eta} dy \\ &= \frac{1}{\int_y b(y) \exp(\eta^T y) dy} \int_y b(y) \exp(\eta^T y) \frac{\partial \eta^T y}{\partial \eta} dy \\ \frac{\partial a(\theta^T x)}{\partial \theta_i} &= \frac{1}{\int_y b(y) \exp(\eta^T y) dy} \int_y b(y) \exp(\eta^T y) \frac{\partial x^T \theta y}{\partial \theta_i} dy \\ &= \frac{1}{\int_y b(y) \exp(\eta^T y) dy} \int_y b(y) \exp(\eta^T y) x_i y dy \\ &= \int_y \frac{b(y) \exp(\eta^T y) dy}{\int_y b(y) \exp(\eta^T y) dy} x_i y dy \\ &= \int_y b(y) \frac{\exp(\eta^T y)}{\exp(a(\eta))} x_i y dy \\ &= \int_y p(y|X; \theta) x_i dy \\ &= x_i \int_y p(y|X; \theta) dy = x_i \mathbb{E}[y|x; \theta] = x_i h_\theta(x) \end{aligned}$$

It follows that:

$$\begin{aligned}\frac{\partial \ell(\theta)}{\partial \theta_i} &= \frac{\partial}{\partial \theta_i} (\theta^T x)^T y - \frac{\partial}{\partial \theta_i} a(\theta^T x) \\ &= x_i y - x_i h_\theta(x) = x_i (y - h_\theta(x))\end{aligned}$$

Therefore, the stochastic gradient ascent on the log likelihood of  $p(y|X; \theta)$  results in the update rule:

$$\theta_i := \theta_i - \alpha (h_\theta(x) - y) x_i$$

### 3. Gaussian discriminant analysis

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

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

(There are two mean vectors  $\mu_1, \mu_{-1}$  but only one covariance matrix  $\Sigma$ .)

Suppose we already fit  $\phi, \Sigma, \mu_1$  and  $\mu_{-1}$  and want to make a prediction at some new query point  $x$ . The posterior distribution of the label  $x$  takes the form:

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

Note that because  $x|y = 1$  and  $x|y = -1$  share the same covariance matrix  $\Sigma$ , the terms in  $\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}}$  cancel one another.

$$p(y = 1|x; \phi, \Sigma, \mu_1, \mu_{-1}) = \frac{1}{1 + \exp\left(\log\left(\frac{\phi}{1-\phi}\right) - \frac{1}{2}(x - \mu_{-1})^T \Sigma^{-1}(x - \mu_{-1}) + \frac{1}{2}(x - \mu_1)^T \Sigma^{-1}(x - \mu_1)\right)}$$

$$p(y = -1|x; \phi, \Sigma, \mu_1, \mu_{-1}) = \frac{1}{1 + \exp\left(\log\left(\frac{1-\phi}{\phi}\right) - \frac{1}{2}(x - \mu_1)^T \Sigma^{-1}(x - \mu_1) + \frac{1}{2}(x - \mu_{-1})^T \Sigma^{-1}(x - \mu_{-1})\right)}$$

More generally,

$$p(y|x; \phi, \Sigma, \mu_1, \mu_{-1}) = \frac{1}{1 + \exp\left[y\left(\log\left(\frac{1-\phi}{\phi}\right) - \underbrace{\frac{1}{2}(x - \mu_{-1})^T \Sigma^{-1}(x - \mu_{-1}) + \frac{1}{2}(x - \mu_1)^T \Sigma^{-1}(x - \mu_1)}_{(1)}\right)\right]}$$

Let  $j = 1$  or  $-1$ .

$$(x - \mu_j)^T \Sigma^j (x - \mu_1) = (x^T \Sigma^{-1} x - 2x^T \Sigma^{-1} u_j + u_j^T \Sigma^{-1} u_j)$$

( $\Sigma^{-1}$  is symmetric therefore  $x^T \Sigma^{-1} u_j = u_j^T \Sigma^{-1} x$ )

$$(1) = \frac{1}{2}(2x^T \Sigma^{-1} \mu_{-1} - \Sigma^{-1} \mu_{-1}^T \mu_{-1} - 2x^T \Sigma^{-1} \mu_1 + \Sigma^{-1} \mu_1^T \mu_1)$$

$$= \frac{1}{2}(-\Sigma^{-1} \mu_{-1}^T \mu_{-1} + \Sigma^{-1} \mu_1^T \mu_1) + (\Sigma^{-1} \mu_{-1} - \Sigma^{-1} \mu_1)^T x$$

Hence,

$$p(y = 1|x; \phi, \Sigma, \mu_1, \mu_{-1}) = \frac{1}{1 + \exp\left(-y\left(\log\left(\frac{\phi}{1-\phi}\right) + \frac{1}{2}(-\Sigma^{-1} \mu_{-1}^T \mu_{-1} + \Sigma^{-1} \mu_1^T \mu_1) + (\Sigma^{-1} \mu_1 - \Sigma^{-1} \mu_{-1})^T x\right)\right)}$$

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

with

$$\theta_0 = \log\left(\frac{\phi}{1-\phi}\right) + \frac{1}{2}(-\Sigma^{-1} \mu_{-1}^T \mu_{-1} + \Sigma^{-1} \mu_1^T \mu_1) \quad \text{and} \quad \theta = \Sigma^{-1} \mu_1 - \Sigma^{-1} \mu_{-1}$$

(b) (proved in (c))

(c) The log likelihood of the data is:

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

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

In order to find the estimator of each of the parameters  $\Sigma, \mu_1, \mu_{-1}$  and  $\phi$ , we compute the gradient of the log likelihood with respect to each parameter:

$$\begin{aligned}
\nabla_{\Sigma} \ell(\phi, \Sigma, \mu_1, \mu_{-1}) &= -\nabla_{\Sigma} m \log((2\pi)^{n/2}|\Sigma|^{1/2}) - \nabla_{\Sigma} \frac{1}{2}(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1}(x^{(i)} - \mu_{y^{(i)}}) \\
\nabla_{\Sigma} m \log((2\pi)^{n/2}|\Sigma|^{1/2}) &= -\frac{m}{2} \nabla_{\Sigma} (|\Sigma|) = \frac{\partial \log(|\Sigma|)}{\partial |\Sigma|} \nabla_{\Sigma} |\Sigma| = \frac{1}{|\Sigma|} (\Sigma^{-T} |\Sigma|) = \Sigma^{-T}
\end{aligned}$$

Since

$$\frac{\partial}{\partial \Sigma_{k,l}} |\Sigma| = \frac{\partial}{\partial \Sigma_{k,l}} \sum_{i=1}^n n(-1)^{i+j} \Sigma_{i,j} |\Sigma_{\setminus i \setminus j}| = (-1)^{k+l} |\Sigma_{k \setminus k, \setminus l}| = (adj(\Sigma))_{l,k}$$

and

$$\nabla_{\Sigma} |\Sigma| = adj(\Sigma)^T = (|\Sigma| \Sigma^{-1})^T = \Sigma^{-T} |\Sigma|$$

For a non-singular matrix  $X$ ,  $\frac{\partial a^T X^{-1} b}{\partial X} = -X^{-T} a b^T X^{-T}$

In our case,

$$\nabla_{\Sigma} \sum_{i=1}^m \frac{1}{2}(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1}(x^{(i)} - \mu_{y^{(i)}}) = -\frac{1}{2} \sum_{i=1}^m \Sigma^{-1}(x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1}$$

and

$$\nabla_{\Sigma} \ell(\phi, \Sigma, \mu_1, \mu_{-1}) = -\frac{m}{2} \Sigma^{-1} + \frac{1}{2} \sum_{i=1}^m \Sigma^{-1} (x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T \Sigma^{-1}$$

At an extremum, the gradient is equal to the zero matrix,

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

We obtain an estimator of the parameter  $\Sigma$ :

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

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

by setting it to the 0 vector,

$$\begin{aligned} 0 &= \sum_{i=1}^m \frac{(1-\phi)1\{y^{(i)} = 1\} - \phi 1\{y^{(i)} = -1\}}{\phi(1-\phi)} \\ &= \sum_{i=1}^m 1\{y^{(i)} = 1\} - \phi 1\{y^{(i)} = 1\} - \phi 1\{y^{(i)} = -1\} \\ &= \sum_{i=1}^m 1\{y^{(i)} = 1\} - \underbrace{\phi(1\{y^{(i)} = 1\} + 1\{y^{(i)} = -1\})}_{=1} = \sum_{i=1}^m 1\{y^{(i)} = 1\} - m\phi \end{aligned}$$

We obtain the estimator of the parameter  $\phi$

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

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

$\Sigma^{-1}$  is symmetric therefore  $\nabla_{(x^{(i)} - \mu_1)}(x^{(i)} - \mu_1)^T \Sigma^{-1}(x^{(i)} - \mu_1) = 2 \Sigma^{-1}(x^{(i)} - \mu_1)$

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

at an extremum the gradient is equal to the zero vector,

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

by pre-multiplying both sides by  $\Sigma$

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

We obtain the estimator of the parameter  $\mu_1$ :

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

conversely an estimator of the parameter  $\mu_{-1}$ ,

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

## 4. Linear invariance of optimization algorithms

We consider using some iterative optimization algorithm (such as Newton's method, or gradient descent) to minimize some continuously differentiable function  $f(x)$  that can be defined as

$$f : \mathbb{R}^n \mapsto \mathbb{R}^m$$

$$x = (x_1, \dots, x_n)^T \rightarrow (f_1(x_1, \dots, x_n)^T, f_2(x_1, \dots, x_n)^T, \dots, f_m(x_1, \dots, x_n)^T)^T$$

where the  $f_i$ -s are continuously differentiable real-valued functions. Let  $A \in \mathbb{R}^{n \times n}$  be some non-singular matrix and let's define a function  $g$ , by  $g(z) = f(Az)$ . Consider we use the same iterative optimization algorithm to optimize  $g$ , (with initialization  $z^{(0)} = \vec{0}$ ). The optimization algorithm is said to be invariable to linear reparameterizations if the values  $z^{(1)}, z^{(2)}, \dots$  satisfy  $z^{(i)} = A^{-1}x^{(i)}$  for all  $i$ .

- (a) We'll show by induction that this is true for the Newton optimization algorithm. In order to avoid tensor notation, we will restrict ourselves to a real valued (multivariable) function  $f$ , which is equivalent to studying the optimization algorithm for each

component  $f_i$  of  $f(x)$ .

The second order approximation of  $f$  near  $x^{(i)}$  is the quadratic function of  $x^{(i)}$  defined by

$$f(x) = f(x^{(i)}) + \nabla f(x^{(i)})^T(x - x^{(i)}) + \frac{1}{2!}(x - x^{(i)})^T Hf(x^{(i)})(x - x^{(i)})$$

Where  $\nabla f(x^{(i)})$  and  $Hf(x^{(i)})$  denote respectively the Gradient and Hessian  $f$  with respect to  $x$ , evaluated at a point  $x^{(i)}$ . We now take the gradient of both sides with respect to  $x$ :

$f(x^{(i)})$  is a constant so its gradient is  $\vec{0}$

$$\nabla_x(\nabla f(x^{(i)})^T(x - x^{(i)})) = \nabla_x f(x^{(i)})$$

because  $f$  is continuously differentiable, its Hessian matrix is symmetric. Then,

$$\nabla_x \left( \frac{1}{2}(x - x^{(i)})^T Hf(x^{(i)})(x - x^{(i)}) \right) = Hf(x^{(i)})$$

At an extremum,  $\nabla_x(f(x)) = 0$ , the update rule follows:

$$x^{(i+1)} = x^{(i)} - (Hf(x^{(i)}))^{-1} \nabla_x f(x^{(i)})$$

because  $g$  is also continuously differentiable, we get the update rule:

$$z^{(i+1)} = z^{(i)} - (Hg(z^{(i)}))^{-1} \nabla_x g(z^{(i)})$$

Base case:  $z^{(0)} = \vec{0} = A^{-1}x^{(0)}$

Induction step: we suppose that for a certain non-zero integer  $i$ , the following is true:

$$(H_i) : z^{(i)} = A^{-1}x^{(i)}$$

Before going any further we must first prove the following equalities:

$$\nabla g(z) = A^T \nabla f(Az) \quad \text{and} \quad Hg(z) = A^T Hf(Az)A$$

$$[\nabla g(z)]_i = \frac{\partial g(z)}{\partial z_i} = \frac{\partial f(Az)}{\partial z_i} = \nabla f(Az) \cdot \frac{\partial f(Az)}{\partial z_i} = \nabla f(Az)A_{\cdot,i}$$

By convention, the gradient is a column vector so:

$$[\nabla g(z)] = A^T \nabla f(Az)$$

Let  $h(z) = \nabla g(z) = A^T \nabla f(Az)$  The Hessian of  $g$  at  $z$  is

$$h'(z) = A^T \nabla^2 f(Az)A$$

Where ' denotes the derivative operator (transpose of the gradient).  
 We can now begin the induction step:

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

Hence,

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

Because it is true for an arbitrary non-zero integer  $i$ , we can conclude that  $\forall i \in \mathbb{N}$ ,  $z^{(i)}$ , the Newton update is invariant to linear transformation.

- (b) Following the same reasoning as in (a),  
 the gradient update of  $x$  can be expressed as, with  $\alpha \in \mathbb{R}$ :

$$x^{(i+1)} = x^{(i)} - \alpha \nabla_f(x^{(i)})$$

On  $z$ ,

$$\begin{aligned}
 z^{(i+1)} &= z^{(i)} - \alpha \nabla_g(z^{(i)}) = z^{(i)} - \alpha \nabla_f(Az^{(i)}) = z^{(i)} - \alpha A^T \nabla_f(x^{(i)}) \\
 Az^{(i+1)} &= \alpha A A^T \nabla_f(x^{(i)}) \neq x^{(i)} - \alpha \nabla_f(x^{(i)}) = x^{(i+1)}
 \end{aligned}$$

(Assuming  $A$  is not the identity matrix.)

**This shows that the gradient descent optimization algorithm is not invariant to linear transformation.**

## 5. Regression for denoising quasar spectra

- (a) Locally weighted linear regression  
 We want to minimize

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

where  $w^{(i)}$  is the weight for a training example ( $i$ ).

Let  $X$  be the  $m$ -by- $d+1$  design matrix that contains the training examples' input values in its rows and  $y$  be an  $m$ -dimensional vector containing all the target values

from the training set:  $X = \begin{bmatrix} - & (x^{(1)})^T & - \\ - & (x^{(2)})^T & - \\ & \vdots & \\ - & (x^{(m)})^T & - \end{bmatrix}$ ;  $y = \begin{bmatrix} - & y^{(1)} & - \\ - & y^{(2)} & - \\ & \vdots & \\ - & y^{(m)} & - \end{bmatrix}$

(i)

$$(X\theta - y)_j = (x^{(j)})^T\theta - y^{(j)}$$

$$[W(X\theta - y)]_i = W_i(X\theta - y) = \sum_{j=1}^m W_{i,j}(x^{(j)})^T\theta - y^{(j)}$$

$$(X\theta - y)_i^T = (x^{(i)})^T\theta - y^{(i)}$$

$$\begin{aligned}(X\theta - y)^T W(X\theta - y) &= \sum_{i=1}^m (X\theta - y)_i^T [W(X\theta - y)]_i \\ &= \sum_{i=1}^m ((x^{(i)})^T\theta - y^{(i)}) \left( \sum_{j=1}^m W_{i,j}(x^{(j)})^T\theta - y^{(j)} \right)\end{aligned}$$

Let

$$W = \frac{1}{2} \begin{bmatrix} w^{(n)} & & \dots & (0) \\ \vdots & \ddots & & \\ (0) & & & w^{(m)} \end{bmatrix}$$

Then,

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

Hence,

$$\begin{aligned}(X\theta - y)^T W(X\theta - y) &= \sum_{i=1}^m ((x^{(i)})^T\theta - y^{(i)}) \left( \frac{w^{(i)}}{2} ((x^{(i)})^T\theta - y^{(i)}) \right) \\ &= \frac{1}{2} \sum_{i=1}^m w^{(i)} ((x^{(i)})^T\theta - y^{(i)})^2 \\ &= J(\theta)\end{aligned}$$