hw2

September 16, 2021

1 Mathematical Foundations of Deep Neural Network

1.1 Homework 2

1.1.1 2017-11362

[1]:
```
# Setting
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

Problem 1: *Logistic regression via SGD.* Use SGD to solve the logistic regression optimization problem

$$\underset{\theta\in\mathbb{R}^p}{\text{minimize}} \quad \frac{1}{N}\sum_{i=1}^{N}\log\left(1+\exp\left(-Y_i X_i^\top \theta\right)\right),$$

where $X_1, \ldots, X_N \in \mathbb{R}^p$, and $Y_1, \ldots, Y_N \in \{-1, 1\}$. Use the data

[2]:
```
N, p = 30, 20
np.random.seed(0)
X = np.random.randn(N, p)
Y = 2*np.random.randint(2, size = N) - 1
```

where $X_1^\top, \ldots, X_N^\top$ are the rows of X.

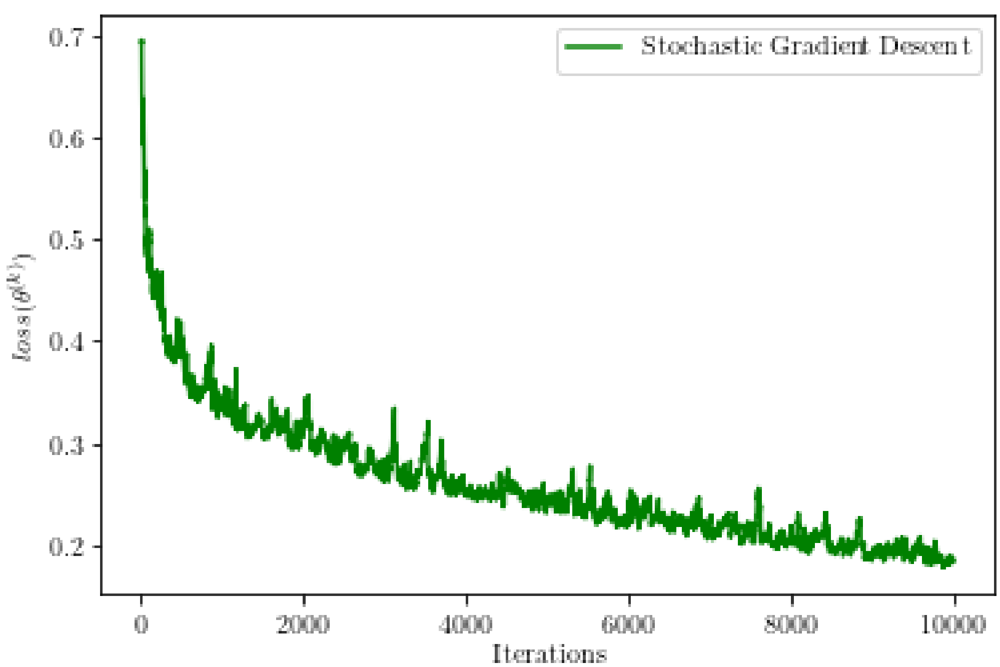
Solution

$$g(\theta) := \nabla_\theta \log(1+\exp(-Y_i X_i^\top \theta)) = \frac{1 - Y_i \exp(-Y_i X_i^\top \theta) X_i}{1+\exp(-Y_i X_i^\top \theta)}$$

$$\theta^{(k+1)} = \theta^{(k)} - \alpha g(\theta^{(k)})$$

[3]:
```
def loss_LR(theta, X=X, Y=Y):
    return np.mean(np.log(1 + np.exp(- Y * np.sum(X * theta, axis=1))))
```

```
def g_LR(theta, ind, X=X, Y=Y):
    Xi, Yi = X[ind,:], Y[ind]
    expo = np.exp(-Yi * np.dot(Xi, theta))
    return - Yi * expo * Xi / (1 + expo)

theta = np.zeros(p) # initial value of theta = 0
alpha = 0.05 # roughly the best value

K = 10000
f_val = []
for _ in range(K):
    ind = np.random.randint(N)
    theta -= alpha * g_LR(theta, ind)
    f_val.append(loss_LR(theta))

plt.rc('text', usetex=True)
plt.rc('font', family='serif')
plt.plot(list(range(K)),f_val, color = "green", label = "Stochastic Gradient␣
 ↪Descent")
plt.xlabel('Iterations')
plt.ylabel(r'$loss(\theta^{(k)})$')
plt.legend()
plt.show()
```



Problem 2: *SVM via SGD.* Use SGD to solve the non-differentiable SVM optimization problem

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \frac{1}{N}\sum_{i=1}^{N} \max\{0, 1 - Y_i X_i^\top \theta\} + \lambda\|\theta\|^2,$$

where $X_1, \dots, X_N \in \mathbb{R}^p$, and $Y_1, \dots, Y_N \in \{-1, 1\}$, and $\lambda = 0.1$. Use the data of Problem 1. Empirically, does the SGD ever encounter a point of non-differentiability?

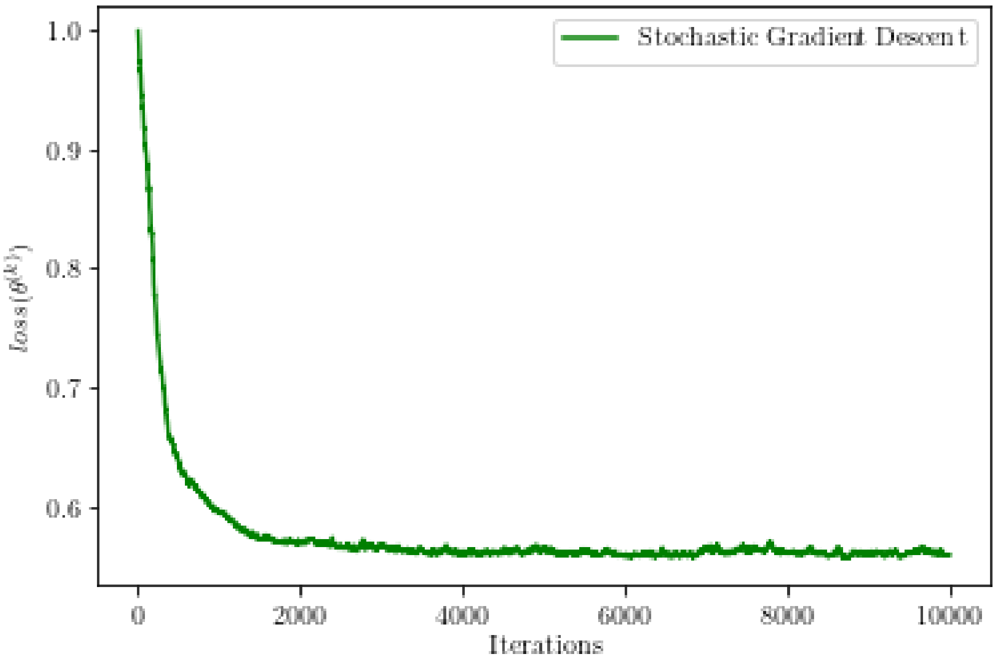
Solution

$$g(\theta) := \nabla_\theta[\max\{0, 1 - Y_i X_i^\top \theta\} + \lambda\|\theta\|^2] = \begin{cases} -Y_i X_i + 2\lambda\theta, & \text{if } 1 - Y_i X_i^\top \theta > 0 \\ 2\lambda\theta, & \text{otherwise} \end{cases}$$

$$\theta^{(k+1)} = \theta^{(k)} - \alpha g(\theta^{(k)})$$

[4]:
```
lam = 0.1

def loss_SVM(theta, X=X, Y=Y, lam=lam):
    return np.mean(np.maximum(0, 1 - Y * np.sum(X * theta, axis=1))) + lam *␣
 ↪theta @ theta

def g_SVM(theta, ind, X=X, Y=Y, lam=lam):
    Xi, Yi = X[ind,:], Y[ind]
    criteria = 1 - Yi * Xi @ theta
    if criteria > 0:
        return -Yi * Xi + 2 * lam * theta
    else:
        if criteria == 0:
            print('SGD encounter a point of non-differentiability!') # check␣
 ↪for non-diff point
        return 2 * lam * theta

theta = np.zeros(p) # initial value of theta = 0
alpha = 0.002 # roughly the best value

K = 10000
f_val = []
for _ in range(K):
    ind = np.random.randint(N)
    theta -= alpha * g_SVM(theta, ind)
    f_val.append(loss_SVM(theta))

plt.rc('text', usetex=True)
plt.rc('font', family='serif')
plt.plot(list(range(K)),f_val, color = "green", label = "Stochastic Gradient␣
 ↪Descent")
```

```
plt.xlabel('Iterations')
plt.ylabel(r'$loss(\theta^{(k)})$')
plt.legend()
plt.show()
```



SGD does not encounter a point of non-differentiability.

Problem 3: Consider the data generated by the Python code

```
[5]: N = 30
np.random.seed(0)
X = np.random.randn(2, N)
y = np.sign(X[0,:] ** 2 + X[1,:]**2 - 0.7)
theta = 0.5
c, s = np.cos(theta), np.sin(theta)
X = np.array([[c, -s], [s, c]]) @ X
X = X + np.array([[1], [1]])
```

Observe (by plotting) that the data is not linearly separable. Consider the transformation

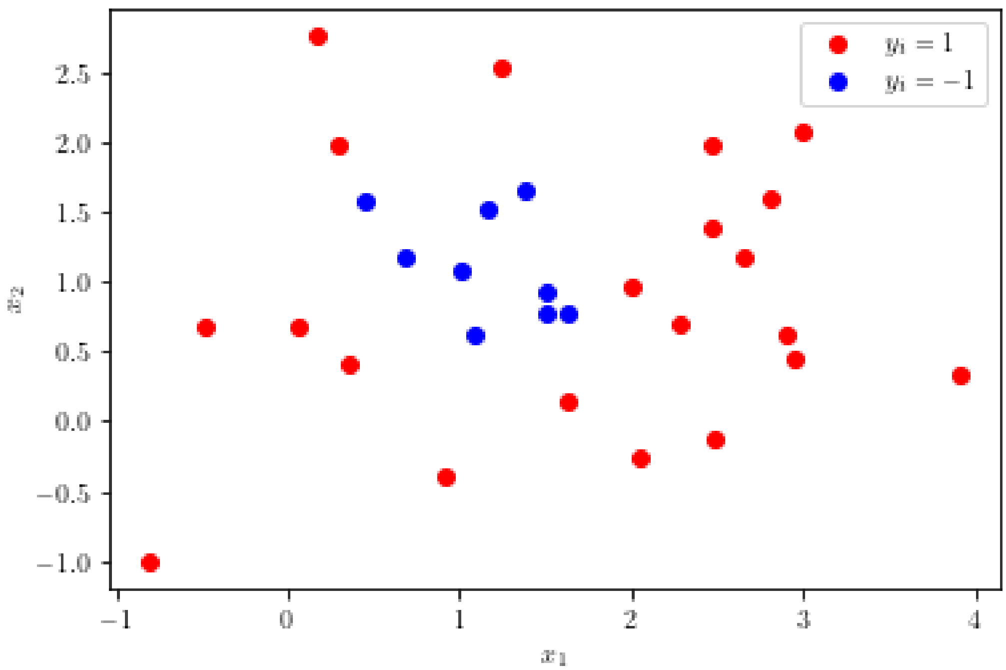
$$\phi\left(\begin{bmatrix} u \\ v \end{bmatrix}\right) = \begin{bmatrix} 1 \\ u \\ u^2 \\ v \\ v^2 \end{bmatrix}$$

Using the logistic regression or SVM, show that the data $\phi(X_1), \ldots, \phi(X_N) \in \mathbb{R}^5$ with labels $Y_1, \ldots, Y_N \in \{-1, +1\}$ is linearly separable. Visualize in $\mathbb{R}^2$ the data and the decision boundary.

Solution

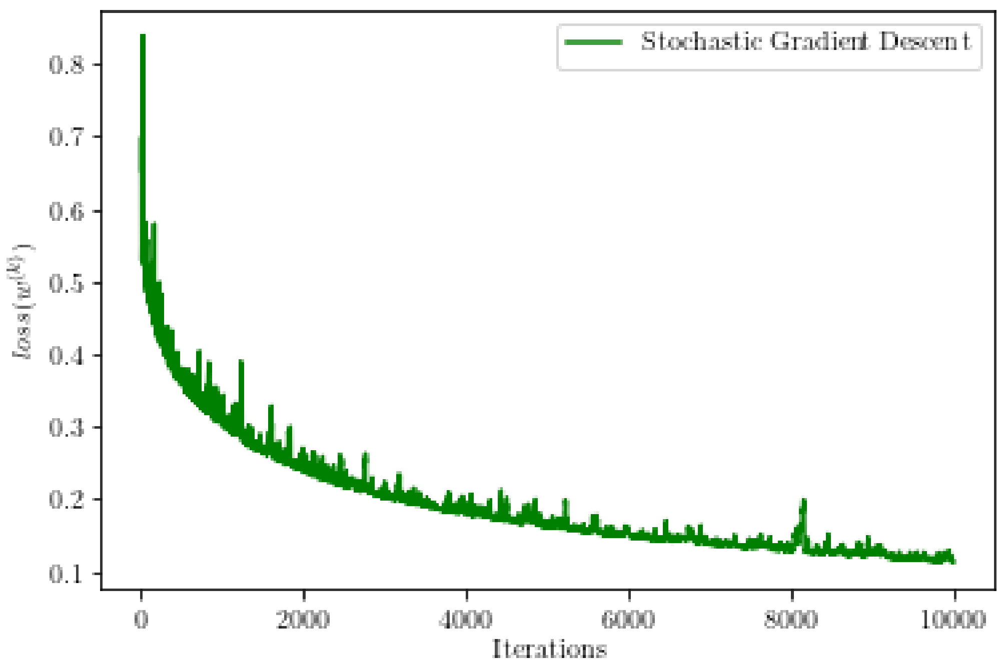
Scatter plot of X (X is not linearly seperable).

[6]:
```
ind1, ind2 = (y == 1), (y == -1)
plt.rc('text', usetex=True)
plt.rc('font', family='serif')
plt.scatter(X[0,ind1], X[1,ind1], color="red", label = r"$y_i = 1$")
plt.scatter(X[0,ind2], X[1,ind2], color="blue", label = r"$y_i = -1$")
plt.xlabel(r'$x_1$')
plt.ylabel(r'$x_2$')
plt.legend()
plt.show()
```

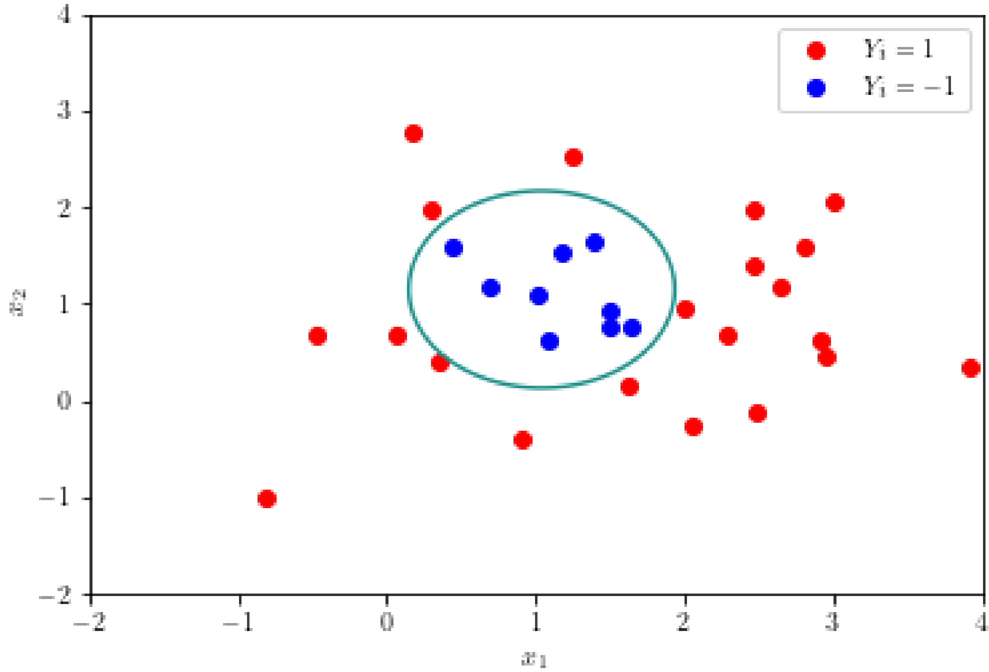


[7]:
```
phiX = np.concatenate((np.ones(N), X[0,:], X[0,:]**2, X[1,:], X[1,:]**2)).
 ↪reshape(5, N).T
w = np.zeros(5) # initial value of theta = 0
alpha = 0.05 # roughly the best value

K = 10000
f_val = []
for _ in range(K):
```

```
    ind = np.random.randint(N)
    w -= alpha * g_LR(w, ind, X=phiX, Y=y)
    f_val.append(loss_LR(w, X=phiX, Y=y))

plt.rc('text', usetex=True)
plt.rc('font', family='serif')
plt.plot(list(range(K)),f_val, color = "green", label = "Stochastic Gradient␣
↪Descent")
plt.xlabel('Iterations')
plt.ylabel(r'$loss(w^{(k)})$')
plt.legend()
plt.show()
```



[8]:
```
xx, yy = np.meshgrid(np.linspace(-2, 4, 1024), np.linspace(-2, 4, 1024))
Z = w[0] + (w[1] * xx + w[2] * xx**2) + (w[3] * yy + w[4] * yy ** 2)

plt.rc('text', usetex=True)
plt.rc('font', family='serif')
plt.scatter(X[0,ind1], X[1,ind1], color="red", label = r"$Y_i = 1$")
plt.scatter(X[0,ind2], X[1,ind2], color="blue", label = r"$Y_i = -1$")
plt.contour(xx, yy, Z, 0)
plt.xlabel(r'$x_1$')
plt.ylabel(r'$x_2$')
plt.legend()
plt.show()
```



Problem 4: *Nonnegativity of KL-divergence.* Show that

$$D_{KL}(p\|q) \geq 0$$

for any probability mass functions $p, q \in \mathbb{R}^n$.

Solution

Claim: $-\log x \geq -x + 1 \quad {}^{\forall}x \geq 0$ (1)

Let $f(x) = -\log x + x - 1$. Then,

$f'(x) = -\frac{1}{x} + 1 = 0 \iff x = 1$

$f(1) = 0,\ \lim_{x\to\infty} f(x) = \lim_{x\to 0+} f(x) = \infty.$

$\therefore f(x) \geq 0 \quad \square.$

Let $X \sim p$ be a random variable. Then,

$$\begin{aligned}
D_{KL}(p\|q) &= \sum_{i=1}^{n} p_i \log\left(\frac{p_i}{q_i}\right) \\
&= \mathbb{E}_p\left[\log\left(\frac{p_X}{q_X}\right)\right] \\
&= \mathbb{E}_p\left[-\log\left(\frac{q_X}{p_X}\right)\right] \\
&\geq \mathbb{E}_p\left[-\frac{q_X}{p_X}+1\right] \quad (\because (1)) \\
&= 1-\sum_{i=1}^{n} p_i \frac{q_i}{p_i} \\
&= 0 \quad (\because \Sigma q_i = 1)
\end{aligned}$$

Problem 5: *Positivity of KL-divergence.* Show that

$$D_{KL}(p\|q) > 0$$

for any probability mass functions $p, q \in \mathbb{R}^n$ such that $p \neq q$.

Solution

From the above claim, equality holds where $-\log x = -x + 1$, which means $x = 1$.

Therefore, $D_{KL}(p\|q) = 0$ where $\frac{q_X}{p_X} = 1$, which means $p = q$.

Problem 6: *Differentiating 2-layer neural networks.* Consider the 2-layer neural network

$$f_\theta(x) = u^\top \sigma(ax+b) = \sum_{j=1}^{p} u_j \sigma(a_j x + b_j),$$

where $a, b, u \in \mathbb{R}^p$ and $\theta = (a_1, \ldots, a_p, b_1, \ldots, b_p, u_1, \ldots, u_p) \in \mathbb{R}^{3p}$. Assume the univariate function $\sigma : \mathbb{R} \to \mathbb{R}$ is differentiable. The notation $\sigma(ax+b)$ means σ is applied elementwise to the vector in $\mathbb{R}^p$. Show that

$$\begin{aligned}
\nabla_u f_\theta(x) &= \sigma(ax+b) \\
\nabla_b f_\theta(x) &= \sigma'(ax+b) \odot u = \operatorname{diag}(\sigma'(ax+b))u \\
\nabla_a f_\theta(x) &= (\sigma'(ax+b) \odot u)x = \operatorname{diag}(\sigma'(ax+b))ux
\end{aligned}$$

where $\sigma'(ax+b)$ means the univariate function σ' is applied elementwise to the vector $ax+b$, $\odot$ denotes the element-wise product, and $\operatorname{diag}(\cdot)$ denotes the diagonal matrix with the diagonal elements equal to the elements of the input vector.

Solution

$\frac{\partial}{\partial u_j} f_\theta(x) = \frac{\partial}{\partial u_j} \sum_{j=1}^{p} u_j \sigma(a_j x + b_j) = \sigma(a_j x + b_j)$

$\Rightarrow \nabla_u f_\theta(x) = \sigma(ax + b)$ ($\because$ jth row of ax is $a_j x$)

$\frac{\partial}{\partial b_j} f_\theta(x) = \frac{\partial}{\partial b_j} \sum_{j=1}^{p} u_j \sigma(a_j x + b_j) = u_j \sigma'(a_j x + b_j)$

$\Rightarrow \nabla_b f_\theta(x) = \sigma'(ax + b) \odot u$

$\frac{\partial}{\partial a_j} f_\theta(x) = \frac{\partial}{\partial a_j} \sum_{j=1}^{p} u_j \sigma(a_j x + b_j) = u_j \sigma'(a_j x + b_j) x$

$\Rightarrow \nabla_a f_\theta(x) = (\sigma'(ax + b) \odot u) x$

Problem 7: *SGD with 2-layer neural networks.*

Solution

[9]:
```
# code from twolayerSGD.py

def f_true(x) :
    return (x-2)*np.cos(x*4)

def sigmoid(x) :
    return 1 / (1 + np.exp(-x))

def sigmoid_prime(x) :
    return sigmoid(x) * (1 - sigmoid(x))

K = 10000
alpha = 0.007
N, p = 30, 50
np.random.seed(0)
a0 = np.random.normal(loc = 0.0, scale = 4.0, size = p)
b0 = np.random.normal(loc = 0.0, scale = 4.0, size = p)
u0 = np.random.normal(loc = 0, scale = 0.05, size = p)
theta = np.concatenate((a0,b0,u0))


X = np.random.normal(loc = 0.0, scale = 1.0, size = N)
Y = f_true(X)

def f_th(theta, x) :
    return np.sum(theta[2*p : 3*p] * sigmoid(theta[0 : p] * np.
 ↪reshape(x,(-1,1)) + theta[p : 2*p]), axis=1)

def diff_f_th(theta, x) :
    #####    implemented part    #####
    a, b, u = theta[ : p], theta[p : 2 * p], theta[2 * p :]
    nabla_u = sigmoid(a * x + b)
```

```
    nabla_b = sigmoid_prime(a * x + b) * u
    nabla_a = x * sigmoid_prime(a * x + b) * u
    return np.concatenate((nabla_a, nabla_b, nabla_u))
    ####################################

xx = np.linspace(-2,2,1024)
plt.plot(X,f_true(X),'rx',label='Data points')
plt.plot(xx,f_true(xx),'r',label='True Fn')

for k in range(K) :
    #####     implemented part     #####
    ind = np.random.randint(N)
    Xi, Yi = X[ind], Y[ind]
    theta -= alpha * diff_f_th(theta, Xi) * (f_th(theta, Xi) - Yi)
    ####################################
    if (k+1)%2000 == 0 :
        plt.plot(xx,f_th(theta, xx),label=f'Learned Fn after {k+1} iterations')

plt.legend()
plt.show()
```