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Logistic Regression

Problem 1

For convenience of showing the expressions, we can define $y_i \in \{0,1\}$ and rewrite $Y_i \in \{-1,1\}$. The y_i here can be transformed back to the space $Y = \{-1,1\}$ by expression $2y_i - 1$. These 2 choices of y_i will not affect the basic of the derivation.

Given a Bernoulli response distribution with $p(y = 1 \mid x; w) = 1/(1 + \exp(-x^T w))$, assume the sample is i.i.d, then the MLE can be written as

$$\begin{aligned} w &= arg \max_w P(y_1, x_1, \ldots, y_n, x_n | w) \\ &= arg \max_w \Pi_{i=1}^n P(y_i | x_i, w) \\ &= arg \max_w \Pi_{i=1}^n p(y = 1 | x; w)^{y_i} (1 - p(y = 1 | x; w))^{1 - y_i} \end{aligned}$$

Take the maximize log likelihood, note $\frac{1}{n}$ is positive,

$$\begin{aligned} w &= arg \max_w log \Pi_{i=1}^n p(y = 1 | x; w)^{y_i} (1 - p(y = 1 | x; w))^{1 - y_i} \\ &= arg \max_w \frac{1}{n} \sum_{i=1}^n (y_i log(p(y = 1 | x; w)) + (1 - y_i) log(1 - p(y = 1 | x; w))) \\ &= arg \max_w -\frac{1}{n} \sum_{i=1}^n (y_i log(1 + exp(-x_i^T w)) + (1 - y_i) log(1 + exp(x_i^T w))) \\ &= arg \max_w -\frac{1}{n} \sum_{i=1}^n (log(1 + exp(-(2y_i - 1) x_i^T w))) \end{aligned}$$

Note since in the beginning, we refine the $y_i \in \{0,1\}$ and y_i can be transformed into $Y \in \{-1,1\}$ by $2y_i - 1$, we can now substitute $2y_i - 1$ in the expression to Y_i, with Y_i denoting the Ys in our dataset D.

The expression is now

$$\begin{aligned} w &= arg \max_w -\frac{1}{n} \sum_{i=1}^n (log(1 + exp(-Y_i x_i^T w))) \\ &= arg \min_w \frac{1}{n} \sum_{i=1}^n (log(1 + exp(-Y_i x_i^T w))) \end{aligned}$$

The ERM with logistic loss is

$$\begin{aligned} w &= arg \min_w \frac{1}{n} \sum_{i=1}^n (l_{logistic}(\hat{y}_i, w), y_i) \\ &= arg \min_w \frac{1}{n} \sum_{i=1}^n (log(1 + exp(-Y_i w^T x_i))) \end{aligned}$$

Therefore the 2 approaches have their objective of the minimization equivalent, and will product the same w with the same optimization algorithm.

Problem 2

Given $p(y = 1 \mid x; w) = 1/(1 + \exp(-x^T w))$, For this problem we have

$$\begin{aligned} P(Y = 1 | x) &= \frac{1}{1 + exp(-x^T w)} \\ P(Y = -1 | x) &= 1 - \frac{1}{1 + exp(-x^T w)} = \frac{exp(-x^T w)}{1 + exp(-x^T w)} \end{aligned}$$

On the decision boundary of the prediction problem we will have

$$\frac{P(Y=1|x)}{P(Y=-1|x)}=1$$

which is equivalent to $P(Y=1|x)=\frac{1}{1+exp(-x^Tw)}=0.5$ or

$$log(\frac{P(Y=1|x)}{P(Y=-1|x)})=0$$

$$log(\frac{\frac{1}{1+exp(-x^Tw)}}{\frac{exp(-x^Tw)}{1+exp(-x^Tw)}})=0$$

Note $1+exp(-x^Tw)$ will not equal to 0, then

$$log(exp(-x^Tw))=0$$
$$x^Tw=0$$

Therefore the boundary of seperating positive and negative is $\{x:x^Tw=0\}$

Problem 3

The likelihood function L of $c\hat{w}$ is

$$L(c\hat{w})=\Pi_{i=1}^n P(y_i|x_i,c\hat{w})$$

If we continue with the Bernoulli response with $p(y=1\mid x;w)=1/(1+\exp(-x^Tw))$, the likelihood function is going to be

$$L(c\hat{w})=\Pi_{i=1}^n p(y=1|x;c\hat{w})^{y_i}(1-p(y=1|x;c\hat{w}))^{1-y_i}$$

Note the log is monotonically increasing and the likelihood is non-negative, to show the problem we can also take derivative of the log maximum likelihood

$$\begin{aligned}l(c\hat{w})&=\sum_{i=1}^n(y_i log(\frac{1}{1+exp(-x_i^Tc\hat{w})})+(1-y_i)log(1-\frac{1}{1+exp(-x_i^Tc\hat{w})}))\\&=-\sum_{i=1}^n(y_i log(1+exp(-x_i^Tc\hat{w}))+(1-y_i)log(1+exp(x_i^Tc\hat{w})))\\&=-\sum_{i=1}^n(log(1+exp(-(2y_i-1)x_i^Tc\hat{w})))\end{aligned}$$

We can take the derivative of $l(c\hat{w})$ with respect to c for a point (x_i,y_i)

$$\begin{aligned}\frac{\partial l(c\hat{w})}{\partial c}&=-\sum_{i=1}^n(log(1+exp(-(2y_i-1)x_i^Tc\hat{w})))\\&=\sum_{i=1}^n\frac{(2y_i-1)x_i^T\hat{w}exp(-(2y_i-1)x_i^Tc\hat{w})}{1+exp(-(2y_i-1)x_i^Tc\hat{w})}\end{aligned}$$

In this expression, the y_i is defined in $\{0,1\}$, so to transform to our definition of the ys in dataset D, we again use the expressions $Y_i\in\{-1,1\}$ and $Y_i=2y_i-1$

$$\frac{\partial l(c\hat{w})}{\partial c}=\sum_{i=1}^n\frac{Y_ix_i^T\hat{w}exp(-Y_ix_i^Tc\hat{w})}{1+exp(-Y_ix_i^Tc\hat{w})}$$

Given that $\hat{w}$ classify all data correctly, $Y_ix_i^T\hat{w}>0$. Meanwhile, $\frac{exp(-Y_ix_i^Tc\hat{w})}{1+exp(-Y_ix_i^Tc\hat{w})}>0$

Therefore,

$$\frac{\partial l(c\hat{w})}{\partial c}>0$$

This expression shows that $l(c\hat{w})$ can increase as c increases, so we can increase the likelihood of the data by $c\hat{w}$.

Problem 4

Here, we can use 2 approaches to show the objective function is convex.

First, the objective function is differentiable and has second derivative. The gradient of the objective function can be written as

$$\begin{aligned}\frac{\partial J(w)}{\partial w}&=\frac{1}{n}\sum_{i=1}^n\frac{exp(-y_iw^Tx_i)(-y_ix_i)}{1+exp(-y_iw^Tx_i)}+2\lambda w\\&=\frac{1}{n}\sum_{i=1}^n(-y_ix_i)(1-\frac{1}{1+exp(-y_iw^Tx_i)})+2\lambda w\end{aligned}$$

The second derivative of the function is

$$\begin{aligned}\frac{\partial^2 J(w)}{\partial w^2} &= \frac{1}{n}\sum_{i=1}^{n} -(y_i x_i)(1+exp(-y_i w^T x_i))^{-2}(exp(-y_i w^T x_i)(-y_i x_i)) + 2\lambda \\ &= \frac{1}{n}\sum_{i=1}^{n}(y_i x_i)^2 \frac{exp(-y_i w^T x_i)}{(1+exp(-y_i w^T x_i))^2} + 2\lambda \\ &> 0\end{aligned}$$

as long as $\lambda > 0 > -\frac{1}{2n}\sum_{i=1}^{n}(y_i x_i)^2 \frac{exp(-y_i w^T x_i)}{(1+exp(-y_i w^T x_i))^2}$

Second, from our convex optimizatio notes on log-sum-exp, $(x_1, \ldots, x_n) \to log(e^{x_1} + \ldots + e^{x_n})$ is convex on R^n.

Thus, $log(1+e^{-y_i w^T x_i}) = log(e^0 + e^{-y_i w^T x_i})$ is convex.

Meanwhile, the l2-norm $||w||^2$ is convex.

Thus, this objective function $J_{logistic}(w)$ is convex.

Problem 5

In [1]:
```
import numpy as np
from scipy.optimize import minimize
from sklearn import preprocessing
import matplotlib.pyplot as plt
```

In [2]:
```
def f_objective(theta, X, y, l2_param):
    '''
    Args:
        theta: 1D numpy array of size num_features
        X: 2D numpy array of size (num_instances, num_features)
        y: 1D numpy array of size num_instances
        l2_param: regularization parameter

    Returns:
        objective: scalar value of objective function
    '''
    n = len(y)
    result = 0
    for i in range(n):
        z = -y[i] * np.dot(theta.T, X[i])
        result += np.logaddexp(0, z)
    result = result/n
    result += l2_param * theta.T @ theta
    return result
```

Problem 6

In [3]:
```python
def fit_logistic_reg(X, y, objective_function, l2_param):
    '''
    Args:
        X: 2D numpy array of size (num_instances, num_features)
        y: 1D numpy array of size num_instances
        objective_function: function returning the value of the objective
        l2_param: regularization parameter

    Returns:
        optimal_theta: 1D numpy array of size num_features
    '''
    def obj_func(theta):
        return objective_function(theta, X, y, l2_param)

    scaler = preprocessing.StandardScaler()
    X = scaler.fit_transform(X)
    X = np.hstack((X, np.ones((X.shape[0], 1))))

    w0 = np.zeros((X.shape[1], 1))
    optimal_theta = minimize(obj_func, w0).x
    return optimal_theta
```

Problem 7

In [4]:
```python
X_train = np.loadtxt('./logistic-code/X_train.txt', delimiter=',')
y_train = np.loadtxt('./logistic-code/y_train.txt', delimiter=',')
X_val = np.loadtxt('./logistic-code/X_val.txt', delimiter=',')
y_val = np.loadtxt('./logistic-code/y_val.txt', delimiter=',')
```

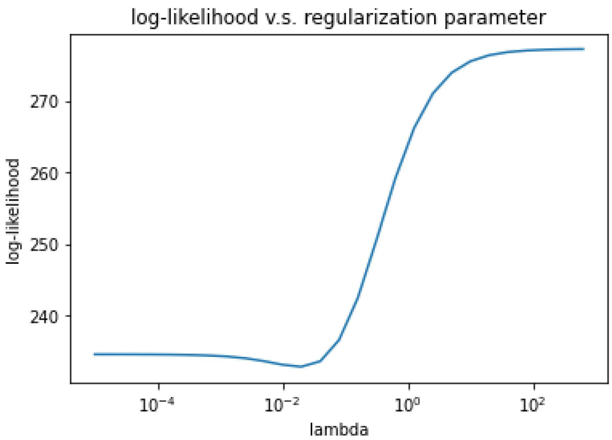
In [5]:
```python
y_train[y_train==0]=-1
y_val[y_val==0]=-1
```

In [6]:
```python
scaler = preprocessing.StandardScaler()
X_val = scaler.fit_transform(X_val)
X_val = np.hstack((X_val, np.ones((X_val.shape[0], 1))))
```

In [8]:
```python
power = np.arange(-5,3,0.3)
l2_param = [10**i for i in power]
opt_theta = []
log_lh = []
for l2 in l2_param:
    res = fit_logistic_reg(X_train, y_train, f_objective, l2)
    ll = len(y_val) * (f_objective(res, X_val, y_val, l2)-l2*res.T@res)
    opt_theta.append(res)
    log_lh.append(ll)
```

In [9]:
```
fig, ax = plt.subplots()
ax.plot(l2_param, log_lh)
ax.set_xscale('log')
ax.set_xlabel('lambda')
ax.set_ylabel('log-likelihood')
ax.set_title('log-likelihood v.s. regularization parameter')
```

Out[9]:
```
Text(0.5, 1.0, 'log-likelihood v.s. regularization parameter')
```



In [10]:
```
ind = int(np.where(log_lh == np.min(log_lh))[0])
print("min log-likelihood = {} and lambda = {}".format(log_lh[ind], l2_param[ind]))
```

```
min log-likelihood = 232.8744022310788 and lambda = 0.019952623149688705
```

Problem 8

In [7]:
```
f_x = np.linspace(0, 1, 10)
#f_x = f_x[1:len(f_x)-1]
tol = 0.1
lamda = 0.02 # the best lambda we found in the previous problem

opt_theta = fit_logistic_reg(X_train, y_train, f_objective, lamda)
```

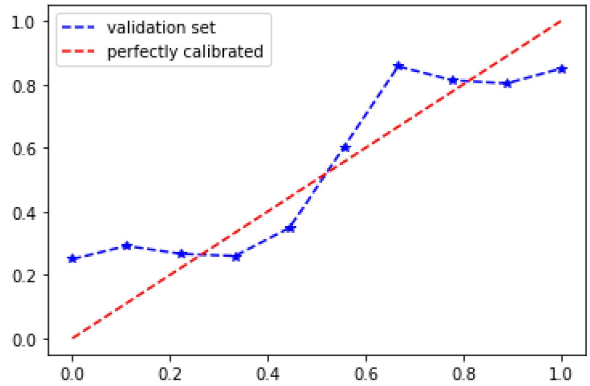
In [8]:
```
def pred_prob(theta, X):
    '''
    Args:
        theta: 1D numpy array of size num_features
        X: 2D numpy array of size (num_instances, num_features)

    Returns:
        result: array of scalar probability of objective function
    '''
    n = X.shape[0]
    result = []
    for i in range(n):
        prob = 1 / (1 + np.exp(-theta.T @ X[i]))
        result.append(prob)
    return np.array(result)
```

In [9]:
```
num = []
prob_array = pred_prob(opt_theta, X_val)
for f in f_x:
    ind = np.where(np.abs(prob_array-f)<tol)
    y_pred = y_val[ind[0]]
    n = np.sum([i == 1 for i in y_pred])/len(ind[0])
    num.append(n)
```

In [114]:
```python
fig, ax = plt.subplots()
ax.plot(f_x, num, '--', label='validation set', color = 'b')
ax.plot(f_x, num, '*', color = 'b')
ax.plot(f_x, f_x, '--', label='perfectly calibrated', color = 'r')
ax.legend(loc='upper left')
```

Out[114]: <matplotlib.legend.Legend at 0x2e203c1beb0>



If we further shrink each group size, the number of samples in each group becomes too small. The samples seem to be calibrated, but since we do not have a large number of samples, the curve of the validation set fluctuates aroung the perfectly calibrated line. Generally, however, logistic regression tend to give well-calibrated predictions by default, as discussed on the scikit-learns's reference page.

Problem 9

By Bayesian Theorem,

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{e^{-NLL_{D(w)}}p(w)}{p(D)}$$

Problem 10

In Bayesian probability theory, if the posterior distributions $p(w|D)$ are in the same probability distribution family as the prior probability distribution $p(w)$, the prior and posterior are conjugate distributions. The prior is then the conjugate prior of the likelihood function $p(D|w)$.

From Bayesian Theorem,

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)}$$

We can calculate the product $p(D|w)p(w)$ and check if the resulting expression can be written in Gaussian form.

The likelihood function of logistic regression is $p(D|w) = e^{\sum_{i=1}^{n}(log(1+exp(-Y_i x_i^T w)))}$

$$\begin{aligned} p(w|D) &= \frac{1}{\sqrt{(2\pi)^k|\Sigma|}}\exp\left(-\frac{1}{2}(w-\mu)^T\Sigma^{-1}(w-\mu)\right)\exp\sum_{i=1}^{n}(log(1+exp(-Y_i x_i^T w))) \\ &= \frac{1}{\sqrt{(2\pi)^k|\Sigma|}}exp(\sum_{i=1}^{n}(-\frac{1}{2\sigma_i}w^2)+log(1+exp(-Y_i x_i^T w))) \end{aligned}$$

This form of expression cannot be written into a gaussian form, and thus this is not a conjugate prior of the likelihood function.

Problem 11

$$\begin{aligned} -log(p(w|D)) &= NLL_{D(w)} - logD(w) + c \\ &= n\hat{R}_n(w) - log(\frac{1}{\sqrt{(2\pi)^k|\Sigma|}}) + \frac{1}{2}(w-\mu)^T\Sigma^{-1}(w-\mu) + c \\ &= n\hat{R}_n(w) + \frac{1}{2}w^T\Sigma^{-1}w + c \end{aligned}$$

Note we have $w\ N(0, \Sigma)$ and c represents an arbitrary constant.

Since we need to find a covariance matrix Σ such that the MAP estimate for w after observing data D is the same as the minimizer of the regularized logistic regression function, we need to have

$$min(-log(p(w|D))) = min(J_{logistic}(w))$$

Therefore, suppose w is the solution we need to have

$$n\hat{R}_n(w) + \frac{1}{2}w^T\Sigma^{-1}w + c = n\hat{R}_n(w) + \lambda n||w||^2$$

This will give $\Sigma = \frac{1}{2n\lambda}I$

Problem 12

In order to have,

$$min(-log(p(w|D))) = min(J_{logistic}(w))$$
$$n\hat{R}_n(w) + \frac{1}{2}w^T\Sigma^{-1}w + c = n\hat{R}_n(w) + \lambda n||w||^2$$
$$n\hat{R}_n(w) + \frac{1}{2}w^T w + c = n\hat{R}_n(w) + \lambda n||w||^2$$

We need to choose $\lambda = \frac{1}{2n}$

Coin Flipping with Partial Observability

Problem 13

By Bayes Theorem,

$$\begin{aligned}
p(x=H|\theta_1,\theta_2) &= \frac{p(x=H,\theta_1,\theta_2)}{p(\theta_1,\theta_2)} \\
&= \frac{p(x=H|Z=H,\theta_1,\theta_2)p(Z=H,\theta_1,\theta_2)+p(x=H|Z=T,\theta_1,\theta_2)p(Z=T,\theta_1,\theta_2)}{p(\theta_1,\theta_2)} \\
&= \frac{p(x=H|Z=H,\theta_1,\theta_2)p(Z=H|\theta_1,\theta_2)p(\theta_1,\theta_2)}{p(\theta_1,\theta_2)} \\
&= p(x=H|Z=H,\theta_1,\theta_2)p(Z=H|\theta_1,\theta_2) \\
&= p(x=H|Z=H,\theta_2)p(Z=H|\theta_1) \\
&= \theta_1\theta_2
\end{aligned}$$

Problem 14

$$\begin{aligned}
L(D_r|\theta_1,\theta_2) &= (\theta_1\theta_2)^{n_h}(1-\theta_1\theta_2)^{n_t} \\
log(L(D_r|\theta_1,\theta_2)) &= n_h log(\theta_1\theta_2) + n_t log(1-\theta_1\theta_2)
\end{aligned}$$

Problem 15

To find the maximum likelihood, since the function is concave, we can take the derivative with respect to θ_1 or θ_2 and then set it to 0. For calculation convinence we can use log likelihood.

$$\begin{aligned}
\frac{\partial log(L(D_r|\theta_1,\theta_2))}{\partial\theta_1} &= \frac{\partial(n_h log(\theta_1\theta_2) + n_t log(1-\theta_1\theta_2))}{\partial\theta_1} \\
&= \frac{n_h\theta_2}{\theta_1\theta_2} + \frac{-n_t\theta_2}{1-\theta_1\theta_2} \\
&= 0
\end{aligned}$$

From the above equation we can get

$$\theta_1\theta_2 = \frac{n_h}{n_h+n_t}$$

We can get a similar expression if we take derivative with respect to θ_2. We can get an equation of the product of $\theta_1\theta_2$, but we cannot estimate θ_1 and θ_2 separately. We need extra dataset to estimate the 2 variables.

Problem 16

$$\begin{aligned} L(\theta_1, \theta_2) &= p(D_r, D_c|\theta_1, \theta_2) \\ &= p(D_c|\theta_1)p(D_r|\theta_1\theta_2) \\ &= \theta_1^{c_h}(1-\theta_1)^{c_t}(\theta_1\theta_2)^{n_h}(1-\theta_1\theta_2)^{n_t} \end{aligned}$$

We can get the log-likelihood of this expression

$$logL(\theta_1, \theta_2) = c_h log(\theta_1) + c_t log(1-\theta_1) + n_h log(\theta_1\theta_2) + n_t log(1-\theta_1\theta_2)$$

Then we can take the derivative and set it to 0

$$\begin{aligned} \frac{\partial logL(\theta_1, \theta_2)}{\partial\theta_1} &= \frac{c_h}{\theta_1} - \frac{c_t}{1-\theta_1} + \frac{n_h\theta_2}{\theta_1\theta_2} - \frac{n_t\theta_2}{1-\theta_1\theta_2} \\ &= \frac{c_h+n_h}{\theta_1} - \frac{c_t}{1-\theta_1} - \frac{n_t\theta_2}{1-\theta_1\theta_2} \\ &= 0 \end{aligned}$$

$$\frac{\partial logL(\theta_1, \theta_2)}{\partial\theta_2} = \frac{n_h\theta_1}{\theta_1\theta_2} - \frac{n_t\theta_1}{1-\theta_1\theta_2} = \frac{n_h}{\theta_2} - \frac{n_t\theta_1}{1-\theta_1\theta_2} = 0$$

Thus we have a system of 2 different equations

$$\begin{cases} \frac{c_h+n_h}{\theta_1} - \frac{c_t}{1-\theta_1} - \frac{n_t\theta_2}{1-\theta_1\theta_2} = 0 \\ \theta_1 = \frac{n_h}{(n_h+n_t)\theta_2} \end{cases}$$

After solving the system of equations, we can have the MLE estimate of θ_1 and θ_2

$$\begin{cases} \theta_2 = \frac{n_h(c_h+c_t)}{(n_h+n_t)c_h} \\ \theta_1 = \frac{c_h}{(c_h+c_t)} \end{cases}$$

Problem 17

Set $D = D_r \cup D_c$, and we can have

$$\begin{aligned} p(\theta_1, \theta_2|D) &= \frac{p(D|\theta_1, \theta_2)p(\theta_1, \theta_2)}{\int_D p(\theta_1, \theta_2, D)\,dx} \\ &\propto (\theta_1\theta_2)^{n_h}(1-\theta_1\theta_2)^{n_t}\theta_1^{c_h}(1-\theta_1)^{c_t}\frac{\Gamma(h+t)}{\Gamma(h)\Gamma(t)}\theta_1^{h-1}(1-\theta_1)^{t-1} \\ &\propto \theta_1^{n_h+h-1+c_h}(1-\theta_1)^{c_t+t-1}\theta_2^{n_h}(1-\theta_1\theta_2)^{n_t} \end{aligned}$$

We can then take the log of the expression,

$$log(p(\theta_1, \theta_2|D)) = (n_h+h-1+c_h)log\theta_1 + (c_t+t-1)log(1-\theta_1) + n_h log\theta_2 + n_t log(1-\theta_1\theta_2) + c$$

Then take the derivative with respect to θ_1 and θ_2 and set to 0,

$$\frac{\partial log(p(\theta_1, \theta_2|D))}{\partial\theta_1} = \frac{(n_h+h-1+c_h)}{\theta_1} + \frac{-(c_t+t-1)}{1-\theta_1} + \frac{-n_t\theta_2}{1-\theta_1\theta_2} = 0$$

$$\frac{\partial log(p(\theta_1, \theta_2|D))}{\partial\theta_2} = \frac{n_h}{\theta_2} + \frac{-n_t\theta_1}{1-\theta_1\theta_2} = 0$$

Then we have 2 equations,

$$\begin{cases} \frac{(n_h+h-1+c_h)}{\theta_1} + \frac{-(c_t+t-1)}{1-\theta_1} + \frac{-n_t\theta_2}{1-\theta_1\theta_2} = 0 \\ \theta_1 = \frac{n_h}{(n_h+n_t)\theta_2} \end{cases}$$

We can solve this system of 2 equations to get

$$\begin{cases} \theta_1 = \frac{h-1+c_h}{h+c_h+c_t+t-2} \\ \theta_2 = \frac{n_h(h+c_h+t+c_t-2)}{(n_h+n_t)(h+c_h-1)} \end{cases}$$