COMP 790-124, HW1

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Problem 1(0.01pt) Open `hw1.tex`, replace "Wile E. Coyote" with your name. Run `pdflatex hw1.tex`, look at hw1.pdf, and confirm that your name is in the right place.

Problem 2(1pt)

1. Plot the sigmoid function in MATLAB using script

   ```
   z = [-5:0.1:5];
   fz = 1./(1 + exp(-z));
   plot(z,fz,'LineWidth',3);
   xlabel('z');ylabel('f(z)'); % we always label axes, yes we do!
   hwplotprep
   print -dpdf sigmoid.pdf
   ```

   Find the resulting figure in file `sigmoid.pdf`. b) In hw1.tex, find the segment of the file that sets up the first figure – it starts with `\begin{figure}` and ends with `\end{figure}`.

2. Inside this segment replace `emptiness.pdf` with `sigmoid.pdf`.

3. Change the text under `\caption` – right now it says "This is emptiness, it earns no points." – to say what the figure is about.

4. Remake hw1.pdf by running in shell/command prompt

   `pdflatex hw1.tex`

   and check that your plot and caption are now in.

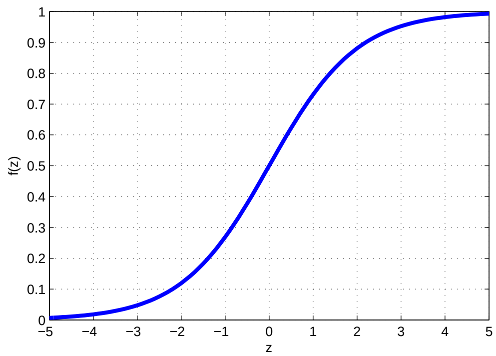

Figure 1: Plot of Sigmoid Function

Problem 3(1pt) Fill in the first derivative and second derivative of sigmoid function in the hw1.tex.

Sigmoid funcion

$$f(z) = \frac{1}{1+e^{-z}}$$

The first derivative

$$\frac{df(z)}{dz} = f(z) * (1 - f(z)) = \frac{1}{e^{z}(1+e^{-z})^2}$$

The second derivative

$$\frac{d^2 f(z)}{dz^2} = \frac{df(z)}{dz} * (1 - 2f(z)) = \frac{1-e^{z}}{e^{2z}(1+e^{-z})^3}$$

Problem 4(1pt) Write a MATLAB function that implements computation of the first derivative of f at a particular point. You just did the math for this.

```
function d = dsigmoid(z)
    % This function computes first derivative of sigmoid function at z
    d = 1 ./ (exp(z) .* (1+exp(-z)).^2);
end
```

Crate a file `dsigmoid.m` that *correctly* computes the first derivative.

Problem 5(1pt) We will use your function `dsigmoid.m` to plot the first derivative.

```
zs = [-5:0.01:5];
for i = 1:length(zs)
```

```
    ds(i) = dsigmoid(zs(i));
end
plot(zs,ds,'LineWidth',3);
xlabel('z');ylabel('df(z)');
hwplotprep
print -dpdf dsigmoid.pdf
```

Find the resulting plot in file `dsigmoid.pdf`. In hw1.tex replace `emptiness.pdf` with `dsigmoid.pdf` . Change the caption in the figure to say what the figure is about. Remake hw1.pdf and check that your plot has made it in.

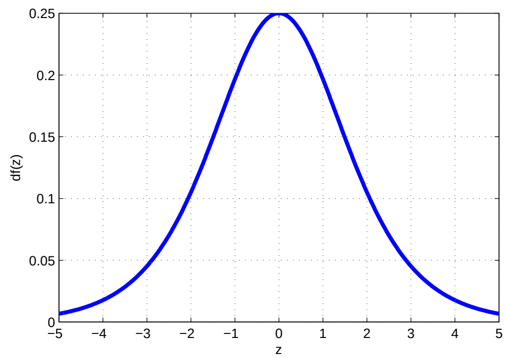

Figure 2: Plot of first order derivative of Sigmoid function

Problem 6(1pt) We can approximate derivatives numerically

$$\frac{df(z)}{dz} \approx \frac{f(z+h) - f(z)}{h}$$

where the right-side of this approximate equality is called *finite difference* approximation. Unlike derivative definition we do not need h to be infinitesimal, just a small value. The numerical approximation of a derivative is tremendously useful trick to check you derivative, gradients, Jacobians, Hessians etc. Make sure that you understand what it does.

We will use this approximation to check your derivatives. Here is a function that computes approximately the derivatives of sigmoid

```
function d = fdsigmoid(z)
f0 = 1/(1 + exp(-z));
f1 = 1/(1 + exp(-(z + 1e-5)));
d = (f1 - f0)/1e-5;
end
```

Save this function into a file names `fdsigmoid.m`.

Try following code in MATLAB

```
zs = randn(100,1);
for i=1:length(zs)
    err(i) = dsigmoid(zs(i)) - fdsigmoid(zs(i));
end
hist(err,30)
hwplotprep
print -dpdf hist.pdf
```

The code above samples 100 normally distributed values and computes the finite differences approximation and the derivative you derived and implemented and then plots histogram of errors.

Find the resulting plot in file `hist.pdf`. In hw1.tex replace `emptiness.pdf` with `hist.pdf` . Change the caption in the figure to say what the figure is about. Remake hw1.pdf and check that your plot has made it in.

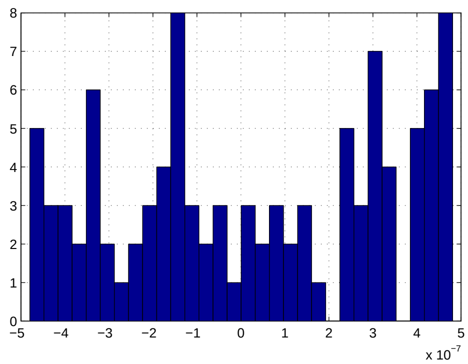

Figure 3: Histogram plot of errors between finite difference approximation and actual first order derivative of Sigmoid function

Remark 1. *The error ranges between* $-4.7959 \times e^{-07}$ *and* $4.8082 \times e^{-07}$.

Problem 7(1pt) From Taylor's theorem (first year calculus) we can obtain

$$f(z+h) = f(z) + \frac{df(z)}{dz}h + \frac{1}{2}\frac{d^2f(z)}{d^2z}h^2 + O(h^3).$$

Derive a bound on the error of the finite differences approximation using the above expression. You can use big O notation to express this bound.

$$\text{Err}(z_0, h) = \left|\frac{f(z_0+h) - f(z_0)}{h} - \frac{df(z_0)}{dz}\right| \leq \frac{1}{2}\frac{d^2f(z_0)}{dz_0{}^2}h + \frac{O(h^3)}{h}$$

Specifically for sigmoid function plug in appropriate derivative on the right hand side of the inequality. If $h = 10^{-5}$ and $z_0 = 0$ the error of the finite difference should be about $\frac{O(h^3)}{h} = 10^{-5\times2} = 10^{-10}$.

Does this agree with the histogram of error that is in the figure above?

Ans. At $h = 10^{-5}$ and $z_0 = 0$ the error of the finite differences and actual derivative (See prob 6 (histogram)) is $9.4645 \times e^{-12}$. As per the above inequality, the difference is 10^{-10}. They are **in agreement** upto a precision of 10 decimal places and the absolute difference between the two is $9.0536 \times e^{-11}$.

Problem 8(1pt) Let

$$f(z) = \frac{1}{1 + \exp\{-z\}} = p \tag{1}$$

express z in terms of p

$$z = \ln\left(\frac{p}{1-p}\right).$$

Now suppose

$$\frac{\exp\{-z\}}{1 + \exp\{-z\}} = q \tag{2}$$

and express z in terms of q

$$z = \ln\left(\frac{1-q}{q}\right).$$

Given Eqs.(1),(2) express q in terms of p

$$q = 1 - p.$$

Express $f(-z)$ in terms of $f(z)$

$$f(-z) = 1 - f(z).$$

Hint: the manipulations that are useful here are either subtraction from 1 (as in $1 - x$), computing inverse (as in $\frac{1}{x}$), and taking logarithm (as in $\log(x)$).

Log of sigmoid

Problem 9(1pt) Let $g(z)$ be log of sigmoid function

$$g(z) = \log\left\{\frac{1}{1 + \exp\{-z\}}\right\}.$$

Compute its derivative and fill it in here

$$\frac{dg(z)}{dz} = \frac{1}{\frac{1}{1+e^{-z}}}\frac{d}{dz}\left(\frac{1}{1+e^{-z}}\right) = (1+e^{-z})\frac{1}{e^{z}(1+e^{-z})^2} = \frac{1}{e^{z}(1+e^{-z})}.$$

$$\frac{dg(z)}{dz} = \frac{1}{1+e^{z}}.$$

Check your derivative by comparing its value to the finite difference approximation.

Problem 10(1pt) Compute second derivative of $g(z)$

$$\frac{d^2 g(z)}{dz^2} = \frac{d}{dz}(\frac{1}{1+e^z}) = -1(1+e^z)^{-2}e^z.$$

$$\frac{d^2 g(z)}{dz^2} = \frac{-e^z}{(1+e^z)^2}.$$

Check the second derivative by comparing its value to the finite difference of the *first* derivatives you computed above.

Problem 11(1pt) Let the dataset be specified by $\mathcal{D} = \{(\mathbf{x}_i, y_i) : i = 1, \dots, n\}$. We specify conditional probability of y

$$p(y|\mathbf{x}_i, \beta_0, \beta) = \frac{1}{1 + \exp\{-y_i(\beta_0 + \langle \beta, \mathbf{x}_i \rangle)\}} \tag{3}$$

Write a matlab function that computes log probability of label y given a vector of features $\mathbf{x}$ and β_0, β.

```
function logP = logProbLogReg(y,X,beta0,beta)
logP = log( .... )
```

Now write a matlab function that uses the above function to compute log probability of label $+1$ for a vector of features $\mathbf{x}$ and β_0, β

```
function predY = predictY(X,beta0,beta)
logProbY = logProgLogReg(X,1,beta0,beta);
if logProbY > ...
    predY = ...
else
    predY = ...
end
```

Problem 12(1pt) Given Eq.(3) we can write out log-likelihood

$$\mathrm{LL}(\beta_0, \beta; \mathcal{D}) = \sum_i \log \frac{1}{1 + \exp\{-y_i(\beta_0 + \langle \beta, \mathbf{x}_i \rangle)\}}. \tag{4}$$

Now using function `logProbLogReg` that you obtained for the previous problem, write a matlab function that computes loglikelihood

```
function val = LogLikLogReg(y,X,beta0,beta)
val = 0;
for i=1:length(y)
   val = val + ...
end
```

Problem 13(1pt) Write a function that computes gradient of log-likelihood of logistic regression Eq.(4)

```
function [dbeta0,dbeta] = dLogLikLogReg(y,X,beta0,beta)
dbeta0 = ...
for i=1:length(beta)
    dbeta(i) = ...
end
```

You can make sure that your implementation is correct using the finite differences trick.

Problem 14(1pt) Implement a gradient ascent algorithm for fitting logistic regression and paste it below.

```
function [beta0,beta] = fitLogReg(y,X)
...
```

Run it with fixed step size $s = 0.01$, for 20 iterations, on data stored in `hw1.mat`. Note that `load hw1.mat` loads the y and X variables, on which you can run by issuing command `[beta0,beta] = fitLogReg(y,X)`. Report resulting β_0, β

```
beta0 = ...
beta0 = ...
```

Problem 15(1pt) Implement estimation of prediction error using cross validation

```
load hw1.mat
rand('seed',1); K = 5; N = length(y);
indices = crossvalind('Kfold',N,K);
for k=1:K
    testX = x(indices == k,:);
    testY = y(indices == k);

    trainX = x(indices ~= k,:);
    trainY = y(indices ~= k,:);

    [beta0,beta] = optimizeLogLikLogReg(trainX,trainY);

    for i=1:length(testY)
        predY = ...
        err(k) = err(k) + ...
    end
end
cvErr = err/length(y);
```

Once done, run this on data stored in `hw1.mat`. The cross-validation estimate of error on that dataset is `answer` .