CS 229

机器学习

(问题及答案)

斯坦福大学

目录

CS 229, Public Course
Problem Set #1: Supervised Learning

1. **Newton's method for computing least squares**

   In this problem, we will prove that if we use Newton's method solve the least squares optimization problem, then we only need one iteration to converge to θ^*.

   (a) Find the Hessian of the cost function $J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})^2$.

   (b) Show that the first iteration of Newton's method gives us $\theta^\star = (X^TX)^{-1}X^T\vec{y}$, the solution to our least squares problem.

2. **Locally-weighted logistic regression**

   In this problem you will implement a locally-weighted version of logistic regression, where we weight different training examples differently according to the query point. The locally-weighted logistic regression problem is to maximize

$$\ell(\theta) = -\frac{\lambda}{2}\theta^T\theta + \sum_{i=1}^{m} w^{(i)}\left[y^{(i)}\log h_\theta(x^{(i)}) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right].$$

   The $-\frac{\lambda}{2}\theta^T\theta$ here is what is known as a regularization parameter, which will be discussed in a future lecture, but which we include here because it is needed for Newton's method to perform well on this task. For the entirety of this problem you can use the value $\lambda = 0.0001$.

   Using this definition, the gradient of $\ell(\theta)$ is given by

$$\nabla_\theta \ell(\theta) = X^T z - \lambda\theta$$

   where $z \in \mathbb{R}^m$ is defined by

$$z_i = w^{(i)}(y^{(i)} - h_\theta(x^{(i)}))$$

   and the Hessian is given by

$$H = X^T D X - \lambda I$$

   where $D \in \mathbb{R}^{m\times m}$ is a diagonal matrix with

$$D_{ii} = -w^{(i)} h_\theta(x^{(i)})(1 - h_\theta(x^{(i)}))$$

   For the sake of this problem you can just use the above formulas, but you should try to derive these results for yourself as well.

   Given a query point x, we choose compute the weights

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

   Much like the locally weighted linear regression that was discussed in class, this weighting scheme gives more when the "nearby" points when predicting the class of a new example.

(a) Implement the Newton-Raphson algorithm for optimizing $\ell(\theta)$ for a new query point x, and use this to predict the class of x.

The `q2/` directory contains data and code for this problem. You should implement the `y = lwlr(X_train, y_train, x, tau)` function in the `lwlr.m` file. This function takes as input the training set (the `X_train` and `y_train` matrices, in the form described in the class notes), a new query point `x` and the weight bandwitdh `tau`. Given this input the function should 1) compute weights $w^{(i)}$ for each training example, using the formula above, 2) maximize $\ell(\theta)$ using Newton's method, and finally 3) output $y = 1\{h_\theta(x) > 0.5\}$ as the prediction.

We provide two additional functions that might help. The `[X_train, y_train] = load_data;` function will load the matrices from files in the `data/` folder. The function `plot_lwlr(X_train, y_train, tau, resolution)` will plot the resulting classifier (assuming you have properly implemented `lwlr.m`). This function evaluates the locally weighted logistic regression classifier over a large grid of points and plots the resulting prediction as blue (predicting $y = 0$) or red (predicting $y = 1$). Depending on how fast your `lwlr` function is, creating the plot might take some time, so we recommend debugging your code with `resolution = 50;` and later increase it to at least 200 to get a better idea of the decision boundary.

(b) Evaluate the system with a variety of different bandwidth parameters τ. In particular, try $\tau = 0.01, 0.050.1, 0.51.0, 5.0$. How does the classification boundary change when varying this parameter? Can you predict what the decision boundary of ordinary (unweighted) logistic regression would look like?

3. **Multivariate least squares**

So far in class, we have only considered cases where our target variable y is a scalar value. Suppose that instead of trying to predict a single output, we have a training set with multiple outputs for each example:

$$\{(x^{(i)}, y^{(i)}),\ i = 1, \ldots, m\},\ x^{(i)} \in \mathbb{R}^n,\ y^{(i)} \in \mathbb{R}^p.$$

Thus for each training example, $y^{(i)}$ is vector-valued, with p entries. We wish to use a linear model to predict the outputs, as in least squares, by specifying the parameter matrix Θ in

$$y = \Theta^T x,$$

where $\Theta \in \mathbb{R}^{n \times p}$.

(a) The cost function for this case is

$$J(\Theta) = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{p} \left((\Theta^T x^{(i)})_j - y_j^{(i)} \right)^2.$$

Write $J(\Theta)$ in matrix-vector notation (i.e., without using any summations). [Hint: Start with the $m \times n$ design matrix

$$X = \begin{bmatrix} — & (x^{(1)})^T & — \\ — & (x^{(2)})^T & — \\ & \vdots & \\ — & (x^{(m)})^T & — \end{bmatrix}$$

and the $m \times p$ target matrix

$$Y = \begin{bmatrix} — & (y^{(1)})^T & — \\ — & (y^{(2)})^T & — \\ & \vdots & \\ — & (y^{(m)})^T & — \end{bmatrix}$$

and then work out how to express $J(\Theta)$ in terms of these matrices.]

(b) Find the closed form solution for Θ which minimizes $J(\Theta)$. This is the equivalent to the normal equations for the multivariate case.

(c) Suppose instead of considering the multivariate vectors $y^{(i)}$ all at once, we instead compute each variable $y_j^{(i)}$ separately for each $j = 1, \ldots, p$. In this case, we have a p individual linear models, of the form

$$y_j^{(i)} = \theta_j^T x^{(i)}, \; j = 1, \ldots, p.$$

(So here, each $\theta_j \in \mathbb{R}^n$). How do the parameters from these p independent least squares problems compare to the multivariate solution?

4. **Naive Bayes**

In this problem, we look at maximum likelihood parameter estimation using the naive Bayes assumption. Here, the input features $x_j, \; j = 1, \ldots, n$ to our model are discrete, binary-valued variables, so $x_j \in \{0, 1\}$. We call $x = [x_1 \; x_2 \; \cdots \; x_n]^T$ to be the input vector. For each training example, our output targets are a single binary-value $y \in \{0, 1\}$. Our model is then parameterized by $\phi_{j|y=0} = p(x_j = 1|y = 0)$, $\phi_{j|y=1} = p(x_j = 1|y = 1)$, and $\phi_y = p(y = 1)$. We model the joint distribution of (x, y) according to

$$\begin{aligned} p(y) &= (\phi_y)^y (1 - \phi_y)^{1-y} \\ p(x|y=0) &= \prod_{j=1}^n p(x_j|y=0) \\ &= \prod_{j=1}^n (\phi_{j|y=0})^{x_j} (1 - \phi_{j|y=0})^{1-x_j} \\ p(x|y=1) &= \prod_{j=1}^n p(x_j|y=1) \\ &= \prod_{j=1}^n (\phi_{j|y=1})^{x_j} (1 - \phi_{j|y=1})^{1-x_j} \end{aligned}$$

(a) Find the joint likelihood function $\ell(\varphi) = \log \prod_{i=1}^m p(x^{(i)}, y^{(i)}; \varphi)$ in terms of the model parameters given above. Here, φ represents the entire set of parameters $\{\phi_y, \; \phi_{j|y=0}, \; \phi_{j|y=1}, \; j = 1, \ldots, n\}$.

(b) Show that the parameters which maximize the likelihood function are the same as those given in the lecture notes; i.e., that

$$\begin{aligned}
\phi_{j|y=0} &= \frac{\sum_{i=1}^m 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 0\}}{\sum_{i=1}^m 1\{y^{(i)} = 0\}} \\
\phi_{j|y=1} &= \frac{\sum_{i=1}^m 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 1\}}{\sum_{i=1}^m 1\{y^{(i)} = 1\}} \\
\phi_y &= \frac{\sum_{i=1}^m 1\{y^{(i)} = 1\}}{m}.
\end{aligned}$$

(c) Consider making a prediction on some new data point x using the most likely class estimate generated by the naive Bayes algorithm. Show that the hypothesis returned by naive Bayes is a linear classifier—i.e., if $p(y = 0|x)$ and $p(y = 1|x)$ are the class probabilities returned by naive Bayes, show that there exists some $\theta \in \mathbb{R}^{n+1}$ such that

$$p(y = 1|x) \geq p(y = 0|x) \text{ if and only if } \theta^T \begin{bmatrix} 1 \\ x \end{bmatrix} \geq 0.$$

(Assume θ_0 is an intercept term.)

5. **Exponential family and the geometric distribution**

(a) Consider the geometric distribution parameterized by ϕ:

$$p(y; \phi) = (1 - \phi)^{y-1}\phi, \; y = 1, 2, 3, \ldots.$$

Show that the geometric distribution is in the exponential family, and give $b(y)$, η, $T(y)$, and $a(\eta)$.

(b) Consider performing regression using a GLM model with a geometric response variable. What is the canonical response function for the family? You may use the fact that the mean of a geometric distribution is given by $1/\phi$.

(c) For a training set $\{(x^{(i)}, y^{(i)});\; i = 1, \ldots, m\}$, 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 goemetric responses y and the canonical response function.

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   (a) Find the Hessian of the cost function $J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})^2$.

   Answer: As shown in the class notes

$$\frac{\partial J(\theta)}{\partial \theta_j} = \sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})x_j^{(i)}.$$

   So

$$\begin{aligned}\frac{\partial^2 J(\theta)}{\partial \theta_j \partial \theta_k} &= \sum_{i=1}^{m}\frac{\partial}{\partial \theta_k}(\theta^T x^{(i)} - y^{(i)})x_j^{(i)} \\ &= \sum_{i=1}^{m} x_j^{(i)} x_k^{(i)} = (X^T X)_{jk}\end{aligned}$$

   Therefore, the Hessian of $J(\theta)$ is $H = X^T X$. This can also be derived by simply applying rules from the lecture notes on Linear Algebra.

   (b) Show that the first iteration of Newton's method gives us $\theta^\star = (X^T X)^{-1} X^T \vec{y}$, the solution to our least squares problem.

   Answer: Given any $\theta^{(0)}$, Newton's method finds $\theta^{(1)}$ according to

$$\begin{aligned}\theta^{(1)} &= \theta^{(0)} - H^{-1}\nabla_\theta J(\theta^{(0)}) \\ &= \theta^{(0)} - (X^T X)^{-1}(X^T X\theta^{(0)} - X^T\vec{y}) \\ &= \theta^{(0)} - \theta^{(0)} + (X^T X)^{-1}X^T\vec{y} \\ &= (X^T X)^{-1}X^T\vec{y}.\end{aligned}$$

   Therefore, no matter what $\theta^{(0)}$ we pick, Newton's method always finds $\theta^\star$ after one iteration.

2. **Locally-weighted logistic regression**

   In this problem you will implement a locally-weighted version of logistic regression, where we weight different training examples differently according to the query point. The locally-weighted logistic regression problem is to maximize

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The $-\frac{\lambda}{2}\theta^T\theta$ here is what is known as a regularization parameter, which will be discussed in a future lecture, but which we include here because it is needed for Newton's method to perform well on this task. For the entirety of this problem you can use the value $\lambda = 0.0001$.

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where $z \in \mathbb{R}^m$ is defined by

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Much like the locally weighted linear regression that was discussed in class, this weighting scheme gives more when the "nearby" points when predicting the class of a new example.

(a) Implement the Newton-Raphson algorithm for optimizing $\ell(\theta)$ for a new query point x, and use this to predict the class of x.

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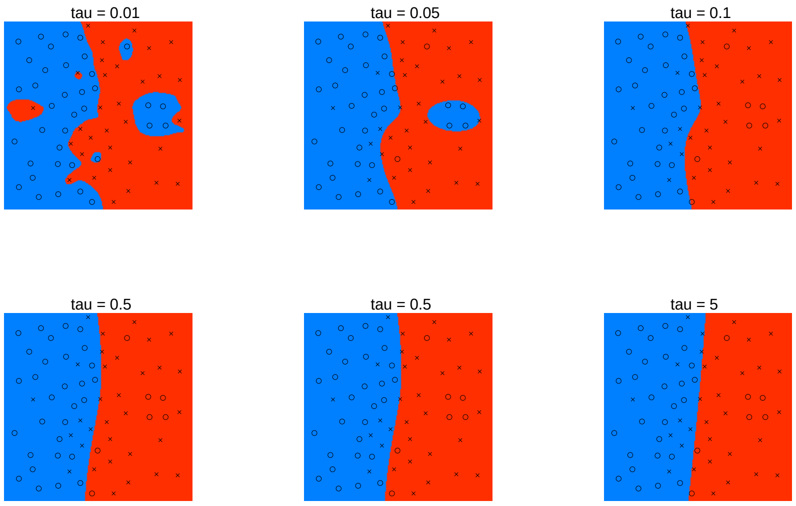
Answer: Our implementation of `lwlr.m`:

```
function y = lwlr(X_train, y_train, x, tau)

m = size(X_train,1);
n = size(X_train,2);
```

```
theta = zeros(n,1);

% compute weights
w = exp(-sum((X_train - repmat(x', m, 1)).^2, 2) / (2*tau));

% perform Newton's method
g = ones(n,1);
while (norm(g) > 1e-6)
  h = 1 ./ (1 + exp(-X_train * theta));
  g = X_train' * (w.*(y_train - h)) - 1e-4*theta;
  H = -X_train' * diag(w.*h.*(1-h)) * X_train - 1e-4*eye(n);
  theta = theta - H \ g;
end

% return predicted y
y = double(x'*theta > 0);
```

(b) Evaluate the system with a variety of different bandwidth parameters τ. In particular, try $\tau = 0.01, 0.050.1, 0.51.0, 5.0$. How does the classification boundary change when varying this parameter? Can you predict what the decision boundary of ordinary (unweighted) logistic regression would look like?

Answer: These are the resulting decision boundaries, for the different values of τ.



For smaller τ, the classifier appears to overfit the data set, obtaining zero training error, but outputting a sporadic looking decision boundary. As τ grows, the resulting decision boundary becomes smoother, eventually converging (in the limit as $\tau \to \infty$ to the unweighted linear regression solution).

3. **Multivariate least squares**

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$$\{(x^{(i)}, y^{(i)}),\ i = 1, \dots, m\},\ x^{(i)} \in \mathbb{R}^n,\ y^{(i)} \in \mathbb{R}^p.$$

Thus for each training example, $y^{(i)}$ is vector-valued, with p entries. We wish to use a linear model to predict the outputs, as in least squares, by specifying the parameter matrix Θ in

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(a) The cost function for this case is

$$J(\Theta) = \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{p}\left((\Theta^T x^{(i)})_j - y_j^{(i)}\right)^2.$$

Write $J(\Theta)$ in matrix-vector notation (i.e., without using any summations). [Hint: Start with the $m \times n$ design matrix

$$X = \begin{bmatrix} — & (x^{(1)})^T & — \\ — & (x^{(2)})^T & — \\ & \vdots & \\ — & (x^{(m)})^T & — \end{bmatrix}$$

and the $m \times p$ target matrix

$$Y = \begin{bmatrix} — & (y^{(1)})^T & — \\ — & (y^{(2)})^T & — \\ & \vdots & \\ — & (y^{(m)})^T & — \end{bmatrix}$$

and then work out how to express $J(\Theta)$ in terms of these matrices.]

Answer: The objective function can be expressed as

$$J(\Theta) = \frac{1}{2}\text{tr}\left((X\Theta - Y)^T(X\Theta - Y)\right).$$

To see this, note that

$$\begin{aligned} J(\Theta) &= \frac{1}{2}\text{tr}\left((X\Theta - Y)^T(X\Theta - Y)\right) \\ &= \frac{1}{2}\sum_i \left(X\Theta - Y)^T(X\Theta - Y)\right)_{ii} \\ &= \frac{1}{2}\sum_i\sum_j (X\Theta - Y)_{ij}^2 \\ &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{p}\left((\Theta^T x^{(i)})_j - y_j^{(i)}\right)^2 \end{aligned}$$

(b) Find the closed form solution for Θ which minimizes $J(\Theta)$. This is the equivalent to the normal equations for the multivariate case.

Answer: First we take the gradient of $J(\Theta)$ with respect to Θ.

$$\begin{aligned}
\nabla_\Theta J(\Theta) &= \nabla_\Theta \left[\frac{1}{2}\text{tr}\left((X\Theta - Y)^T(X\Theta - Y)\right)\right] \\
&= \nabla_\Theta \left[\frac{1}{2}\text{tr}\left(\Theta^T X^T X\Theta - \Theta^T X^T Y - Y^T X\Theta - Y^T T\right)\right] \\
&= \frac{1}{2}\nabla_\Theta \left[\text{tr}(\Theta^T X^T X\Theta) - \text{tr}(\Theta^T X^T Y) - \text{tr}(Y^T X\Theta) + \text{tr}(Y^T Y)\right] \\
&= \frac{1}{2}\nabla_\Theta \left[\text{tr}(\Theta^T X^T X\Theta) - 2\text{tr}(Y^T X\Theta) + \text{tr}(Y^T Y)\right] \\
&= \frac{1}{2}\left[X^T X\Theta + X^T X\Theta - 2X^T Y\right] \\
&= X^T X\Theta - X^T Y
\end{aligned}$$

Setting this expression to zero we obtain

$$\Theta = (X^T X)^{-1} X^T Y.$$

This looks very similar to the closed form solution in the univariate case, except now Y is a $m \times p$ matrix, so then Θ is also a matrix, of size $n \times p$.

(c) Suppose instead of considering the multivariate vectors $y^{(i)}$ all at once, we instead compute each variable $y_j^{(i)}$ separately for each $j = 1, \ldots, p$. In this case, we have a p individual linear models, of the form

$$y_j^{(i)} = \theta_j^T x^{(i)},\ j = 1, \ldots, p.$$

(So here, each $\theta_j \in \mathbb{R}^n$). How do the parameters from these p independent least squares problems compare to the multivariate solution?

Answer: This time, we construct a set of vectors

$$\vec{y}_j = \begin{bmatrix} y_j^{(1)} \\ y_j^{(2)} \\ \vdots \\ y_j^{(m)} \end{bmatrix},\ j = 1, \ldots, p.$$

Then our j-th linear model can be solved by the least squares solution

$$\theta_j = (X^T X)^{-1} X^T \vec{y}_j.$$

If we line up our θ_j, we see that we have the following equation:

$$\begin{aligned}
[\theta_1\ \theta_2\ \cdots\ \theta_p] &= \left[(X^T X)^{-1} X^T \vec{y}_1\ (X^T X)^{-1} X^T \vec{y}_2\ \cdots\ (X^T X)^{-1} X^T \vec{y}_p\right] \\
&= (X^T X)^{-1} X^T \left[\vec{y}_1\ \vec{y}_2\ \cdots\ \vec{y}_p\right] \\
&= (X^T X)^{-1} X^T Y \\
&= \Theta.
\end{aligned}$$

Thus, our p individual least squares problems give the exact same solution as the multivariate least squares.

4. **Naive Bayes**

   In this problem, we look at maximum likelihood parameter estimation using the naive Bayes assumption. Here, the input features $x_j,\ j = 1, \ldots, n$ to our model are discrete, binary-valued variables, so $x_j \in \{0, 1\}$. We call $x = [x_1\ x_2\ \cdots\ x_n]^T$ to be the input vector. For each training example, our output targets are a single binary-value $y \in \{0, 1\}$. Our model is then parameterized by $\phi_{j|y=0} = p(x_j = 1|y = 0)$, $\phi_{j|y=1} = p(x_j = 1|y = 1)$, and $\phi_y = p(y = 1)$. We model the joint distribution of (x, y) according to

$$\begin{aligned}
p(y) &= (\phi_y)^y(1-\phi_y)^{1-y} \\
p(x|y=0) &= \prod_{j=1}^{n} p(x_j|y=0) \\
&= \prod_{j=1}^{n} (\phi_{j|y=0})^{x_j}(1-\phi_{j|y=0})^{1-x_j} \\
p(x|y=1) &= \prod_{j=1}^{n} p(x_j|y=1) \\
&= \prod_{j=1}^{n} (\phi_{j|y=1})^{x_j}(1-\phi_{j|y=1})^{1-x_j}
\end{aligned}$$

   (a) Find the joint likelihood function $\ell(\varphi) = \log \prod_{i=1}^{m} p(x^{(i)}, y^{(i)}; \varphi)$ in terms of the model parameters given above. Here, φ represents the entire set of parameters $\{\phi_y,\ \phi_{j|y=0},\ \phi_{j|y=1},\ j = 1, \ldots, n\}$.
   Answer:

$$\begin{aligned}
\ell(\varphi) &= \log \prod_{i=1}^{m} p(x^{(i)}, y^{(i)}; \varphi) \\
&= \log \prod_{i=1}^{m} p(x^{(i)}|y^{(i)}; \varphi)p(y^{(i)}; \varphi) \\
&= \log \prod_{i=1}^{m} \left(\prod_{j=1}^{n} p(x_j^{(i)}|y^{(i)}; \varphi) \right) p(y^{(i)}; \varphi) \\
&= \sum_{i=1}^{m} \left(\log p(y^{(i)}; \varphi) + \sum_{j=1}^{n} \log p(x_j^{(i)}|y^{(i)}; \varphi) \right) \\
&= \sum_{i=1}^{m} \Bigg[y^{(i)} \log \phi_y + (1-y^{(i)}) \log(1-\phi_y) \\
&\qquad + \sum_{j=1}^{n} \left(x_j^{(i)} \log \phi_{j|y^{(i)}} + (1-x_j^{(i)}) \log(1-\phi_{j|y^{(i)}}) \right) \Bigg]
\end{aligned}$$

   (b) Show that the parameters which maximize the likelihood function are the same as those given in the lecture notes; i.e., that

$$\begin{aligned}
\phi_{j|y=0} &= \frac{\sum_{i=1}^m 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 0\}}{\sum_{i=1}^m 1\{y^{(i)} = 0\}} \\
\phi_{j|y=1} &= \frac{\sum_{i=1}^m 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 1\}}{\sum_{i=1}^m 1\{y^{(i)} = 1\}} \\
\phi_y &= \frac{\sum_{i=1}^m 1\{y^{(i)} = 1\}}{m}.
\end{aligned}$$

Answer: The only terms in $\ell(\varphi)$ which have non-zero gradient with respect to $\phi_{j|y=0}$ are those which include $\phi_{j|y^{(i)}}$. Therefore,

$$\begin{aligned}
\nabla_{\phi_{j|y=0}}\ell(\varphi) &= \nabla_{\phi_{j|y=0}} \sum_{i=1}^m \left(x_j^{(i)} \log \phi_{j|y^{(i)}} + (1-x_j^{(i)}) \log(1-\phi_{j|y^{(i)}})\right) \\
&= \nabla_{\phi_{j|y=0}} \sum_{i=1}^m \left(x_j^{(i)} \log(\phi_{j|y=0}) 1\{y^{(i)} = 0\}\right. \\
&\qquad \left. + (1-x_j^{(i)}) \log(1-\phi_{j|y=0}) 1\{y^{(i)} = 0\}\right) \\
&= \sum_{i=1}^m \left(x_j^{(i)} \frac{1}{\phi_{j|y=0}} 1\{y^{(i)} = 0\} - (1-x_j^{(i)}) \frac{1}{1-\phi_{j|y=0}} 1\{y^{(i)} = 0\}\right).
\end{aligned}$$

Setting $\nabla_{\phi_{j|y=0}}\ell(\varphi) = 0$ gives

$$\begin{aligned}
0 &= \sum_{i=1}^m \left(x_j^{(i)} \frac{1}{\phi_{j|y=0}} 1\{y^{(i)} = 0\} - (1-x_j^{(i)}) \frac{1}{1-\phi_{j|y=0}} 1\{y^{(i)} = 0\}\right) \\
&= \sum_{i=1}^m \left(x_j^{(i)}(1-\phi_{j|y=0}) 1\{y^{(i)} = 0\} - (1-x_j^{(i)}) \phi_{j|y=0} 1\{y^{(i)} = 0\}\right) \\
&= \sum_{i=1}^m \left((x_j^{(i)} - \phi_{j|y=0}) 1\{y^{(i)} = 0\}\right) \\
&= \sum_{i=1}^m \left(x_j^{(i)} \cdot 1\{y^{(i)} = 0\}\right) - \phi_{j|y=0} \sum_{i=1}^m 1\{y^{(i)} = 0\} \\
&= \sum_{i=1}^m \left(1\{x_j^{(i)} = 1 \wedge y^{(i)} = 0\}\right) - \phi_{j|y=0} \sum_{i=1}^m 1\{y^{(i)} = 0\}.
\end{aligned}$$

We then arrive at our desired result

$$\phi_{j|y=0} = \frac{\sum_{i=1}^m 1\{x_j^{(i)} = 1 \wedge y^{(i)} = 0\}}{\sum_{i=1}^m 1\{y^{(i)} = 0\}}$$

The solution for $\phi_{j|y=1}$ proceeds in the identical manner.

To solve for ϕ_y,

$$\begin{aligned}\nabla_{\phi_y}\ell(\varphi) &= \nabla_{\phi_y}\sum_{i=1}^{m}\left(y^{(i)}\log\phi_y + (1-y^{(i)})\log(1-\phi_y)\right)\\ &= \sum_{i=1}^{m}\left(y^{(i)}\frac{1}{\phi_y} - (1-y^{(i)})\frac{1}{1-\phi_y}\right)\end{aligned}$$

Then setting $\nabla_{\phi_y}=0$ gives us

$$\begin{aligned}0 &= \sum_{i=1}^{m}\left(y^{(i)}\frac{1}{\phi_y} - (1-y^{(i)})\frac{1}{1-\phi_y}\right)\\ &= \sum_{i=1}^{m}\left(y^{(i)}(1-\phi_y) - (1-y^{(i)})\phi_y\right)\\ &= \sum_{i=1}^{m}y^{(i)} - \sum_{i=1}^{m}\phi_y.\end{aligned}$$

Therefore,

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

(c) Consider making a prediction on some new data point x using the most likely class estimate generated by the naive Bayes algorithm. Show that the hypothesis returned by naive Bayes is a linear classifier—i.e., if $p(y=0|x)$ and $p(y=1|x)$ are the class probabilities returned by naive Bayes, show that there exists some $\theta\in\mathbb{R}^{n+1}$ such that

$$p(y=1|x)\geq p(y=0|x) \text{ if and only if } \theta^T\left[\begin{array}{c}1\\x\end{array}\right]\geq 0.$$

(Assume θ_0 is an intercept term.)

Answer:

$$\begin{aligned}&p(y=1|x)\geq p(y=0|x)\\ \Longleftrightarrow\ &\frac{p(y=1|x)}{p(y=0|x)}\geq 1\\ \Longleftrightarrow\ &\frac{\left(\prod_{j=1}^{n}p(x_j|y=1)\right)p(y=1)}{\left(\prod_{j=1}^{n}p(x_j|y=0)\right)p(y=0)}\geq 1\\ \Longleftrightarrow\ &\frac{\left(\prod_{j=1}^{n}(\phi_{j|y=0})^{x_j}(1-\phi_{j|y=0})^{1-x_j}\right)\phi_y}{\left(\prod_{j=1}^{n}(\phi_{j|y=1})^{x_j}(1-\phi_{j|y=1})^{1-x_j}\right)(1-\phi_y)}\geq 1\\ \Longleftrightarrow\ &\sum_{j=1}^{n}\left(x_j\log\left(\frac{\phi_{j|y=1}}{\phi_{j|y=0}}\right)+(1-x_j)\log\left(\frac{1-\phi_{j|y=0}}{1-\phi_j|y=0}\right)\right)+\log\left(\frac{\phi_y}{1-\phi_y}\right)\geq 0\\ \Longleftrightarrow\ &\sum_{j=1}^{n}x_j\log\left(\frac{(\phi_{j|y=1})(1-\phi_{j|y=0})}{(\phi_{j|y=0})(1-\phi_{j|y=1})}\right)+\sum_{j=1}^{n}\log\left(\frac{1-\phi_{j|y=1}}{1-\phi_{j|y=0}}\right)+\log\left(\frac{\phi_y}{1-\phi_y}\right)\geq 0\\ \Longleftrightarrow\ &\theta^T\left[\begin{array}{c}1\\x\end{array}\right]\geq 0,\end{aligned}$$

where

$$\begin{aligned}\theta_0 &= \sum_{j=1}^{n} \log\left(\frac{1-\phi_{j|y=1}}{1-\phi_{j|y=0}}\right) + \log\left(\frac{\phi_y}{1-\phi_y}\right)\\ \theta_j &= \log\left(\frac{(\phi_{j|y=1})(1-\phi_{j|y=0})}{(\phi_{j|y=0})(1-\phi_{j|y=1})}\right),\ j = 1,\ldots,n.\end{aligned}$$

5. **Exponential family and the geometric distribution**

(a) Consider the geometric distribution parameterized by ϕ:

$$p(y;\phi) = (1-\phi)^{y-1}\phi,\ y = 1,2,3,\ldots.$$

Show that the geometric distribution is in the exponential family, and give $b(y)$, η, $T(y)$, and $a(\eta)$.

Answer:

$$\begin{aligned}p(y;\phi) &= (1-\phi)^{y-1}\phi\\ &= \exp\left[\log(1-\phi)^{y-1} + \log\phi\right]\\ &= \exp\left[(y-1)\log(1-\phi) + \log\phi\right]\\ &= \exp\left[y\log(1-\phi) - \log\left(\frac{1-\phi}{\phi}\right)\right]\end{aligned}$$

Then

$$\begin{aligned}b(y) &= 1\\ \eta &= \log(1-\phi)\\ T(y) &= y\\ a(\eta) &= \log\left(\frac{1-\phi}{\phi}\right) = \log\left(\frac{e^\eta}{1-e^\eta}\right),\end{aligned}$$

where the last line follows becuase $\eta = \log(1-\phi) \Rightarrow e^\eta = 1-\phi \Rightarrow \phi = 1-e^\eta$.

(b) Consider performing regression using a GLM model with a geometric response variable. What is the canonical response function for the family? You may use the fact that the mean of a geometric distribution is given by $1/\phi$.

Answer:

$$g(\eta) = E[y;\phi] = \frac{1}{\phi} = \frac{1}{1-e^\eta}.$$

(c) For a training set $\{(x^{(i)}, y^{(i)});\ i = 1,\ldots,m\}$, 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 goemetric responses y and the canonical response function.

Answer: The log-likelihood of an example $(x^{(i)}, y^{(i)})$ is defined as $\ell(\theta) = \log p(y^{(i)}|x^{(i)};\theta)$. To derive the stochastic gradient ascent rule, use the results from previous parts and the standard GLM assumption that $\eta = \theta^T x$.

$$\begin{aligned}
\ell_i(\theta) &= \log\left[\exp\left(\theta^T x^{(i)} \cdot y^{(i)} - \log\left(\frac{e^{\theta^T x^{(i)}}}{1-e^{\theta^T x^{(i)}}}\right)\right)\right] \\
&= \log\left[\exp\left(\theta^T x^{(i)} \cdot y^{(i)} - \log\left(\frac{1}{e^{-\theta^T x^{(i)}}-1}\right)\right)\right] \\
&= \theta^T x^{(i)} \cdot y^{(i)} + \log\left(e^{-\theta^T x^{(i)}} - 1\right) \\
\frac{\partial}{\partial\theta_j}\ell_i(\theta) &= x_j^{(i)} y^{(i)} + \frac{e^{-\theta^T x^{(i)}}}{e^{-\theta^T x^{(i)}}-1}(-x_j^{(i)}) \\
&= x_j^{(i)} y^{(i)} - \frac{1}{1-e^{-\theta^T x^{(i)}}} x_j^{(i)} \\
&= \left(y^{(i)} - \frac{1}{1-e^{\theta^T x^{(i)}}}\right) x_j^{(i)}.
\end{aligned}$$

Thus the stochastic gradient ascent update rule should be

$$\theta_j := \theta_j + \alpha \frac{\partial \ell_i(\theta)}{\partial \theta_j},$$

which is

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - \frac{1}{1-e^{\theta^T x^{(i)}}}\right) x_j^{(i)}.$$

CS 229, Public Course
Problem Set #2: Kernels, SVMs, and Theory

1. **Kernel ridge regression**

   In contrast to ordinary least squares which has a cost function

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

   we can also add a term that penalizes large weights in θ. In *ridge regression*, our least squares cost is regularized by adding a term $\lambda\|\theta\|^2$, where $\lambda > 0$ is a fixed (known) constant (regularization will be discussed at greater length in an upcoming course lecutre). The ridge regression cost function is then

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

   (a) Use the vector notation described in class to find a closed-form expreesion for the value of θ which minimizes the ridge regression cost function.

   (b) Suppose that we want to use kernels to implicitly represent our feature vectors in a high-dimensional (possibly infinite dimensional) space. Using a feature mapping ϕ, the ridge regression cost function becomes

   $$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(\theta^T \phi(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2}\|\theta\|^2.$$

   Making a prediction on a new input x_{new} would now be done by computing $\theta^T\phi(x_{\text{new}})$. Show how we can use the "kernel trick" to obtain a closed form for the prediction on the new input without ever explicitly computing $\phi(x_{\text{new}})$. You may assume that the parameter vector θ can be expressed as a linear combination of the input feature vectors; i.e., $\theta = \sum_{i=1}^{m}\alpha_i\phi(x^{(i)})$ for some set of parameters α_i.
   [Hint: You may find the following identity useful:

   $$(\lambda I + BA)^{-1}B = B(\lambda I + AB)^{-1}.$$

   If you want, you can try to prove this as well, though this is not required for the problem.]

2. **ℓ_2 norm soft margin SVMs**

   In class, we saw that if our data is not linearly separable, then we need to modify our support vector machine algorithm by introducing an error margin that must be minimized. Specifically, the formulation we have looked at is known as the ℓ_1 norm soft margin SVM. In this problem we will consider an alternative method, known as the ℓ_2 norm soft margin SVM. This new algorithm is given by the following optimization problem (notice that the slack penalties are now squared):

   $$\begin{array}{ll} \min_{w,b,\xi} & \frac{1}{2}\|w\|^2 + \frac{C}{2}\sum_{i=1}^{m}\xi_i^2 \\ \text{s.t.} & y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i,\ i = 1, \ldots, m \end{array}.$$

(a) Notice that we have dropped the $\xi_i \geq 0$ constraint in the ℓ_2 problem. Show that these non-negativity constraints can be removed. That is, show that the optimal value of the objective will be the same whether or not these constraints are present.

(b) What is the Lagrangian of the ℓ_2 soft margin SVM optimization problem?

(c) Minimize the Lagrangian with respect to w, b, and ξ by taking the following gradients: $\nabla_w \mathcal{L}$, $\frac{\partial \mathcal{L}}{\partial b}$, and $\nabla_\xi \mathcal{L}$, and then setting them equal to 0. Here, $\xi = [\xi_1, \xi_2, \ldots, \xi_m]^T$.

(d) What is the dual of the ℓ_2 soft margin SVM optimization problem?

3. **SVM with Gaussian kernel**

Consider the task of training a support vector machine using the Gaussian kernel $K(x,z) = \exp(-\|x-z\|^2/\tau^2)$. We will show that as long as there are no two identical points in the training set, we can always find a value for the bandwidth parameter τ such that the SVM achieves zero training error.

(a) Recall from class that the decision function learned by the support vector machine can be written as

$$f(x) = \sum_{i=1}^{m} \alpha_i y^{(i)} K(x^{(i)}, x) + b.$$

Assume that the training data $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$ consists of points which are separated by at least a distance of ϵ; that is, $||x^{(j)} - x^{(i)}|| \geq \epsilon$ for any $i \neq j$. Find values for the set of parameters $\{\alpha_1, \ldots, \alpha_m, b\}$ and Gaussian kernel width τ such that $x^{(i)}$ is correctly classified, for all $i = 1, \ldots, m$. [Hint: Let $\alpha_i = 1$ for all i and $b = 0$. Now notice that for $y \in \{-1, +1\}$ the prediction on $x^{(i)}$ will be correct if $|f(x^{(i)}) - y^{(i)}| < 1$, so find a value of τ that satisfies this inequality for all i.]

(b) Suppose we run a SVM with slack variables using the parameter τ you found in part (a). Will the resulting classifier necessarily obtain zero training error? Why or why not? A short explanation (without proof) will suffice.

(c) Suppose we run the SMO algorithm to train an SVM with slack variables, under the conditions stated above, using the value of τ you picked in the previous part, and using some arbitrary value of C (which you do not know beforehand). Will this necessarily result in a classifier that achieve zero training error? Why or why not? Again, a short explanation is sufficient.

4. **Naive Bayes and SVMs for Spam Classification**

In this question you'll look into the Naive Bayes and Support Vector Machine algorithms for a spam classification problem. However, instead of implementing the algorithms yourself, you'll use a freely available machine learning library. There are many such libraries available, with different strengths and weaknesses, but for this problem you'll use the WEKA machine learning package, available at `http://www.cs.waikato.ac.nz/ml/weka/`. WEKA implements many standard machine learning algorithms, is written in Java, and has both a GUI and a command line interface. It is not the best library for very large-scale data sets, but it is very nice for playing around with many different algorithms on medium size problems.

You can download and install WEKA by following the instructions given on the website above. To use it from the command line, you first need to install a java runtime environment, then add the `weka.jar` file to your `CLASSPATH` environment variable. Finally, you can call WEKA using the command:

```
java <classifier> -t <training file> -T <test file>
```

For example, to run the Naive Bayes classifier (using the multinomial event model) on our provided spam data set by running the command:

```
java weka.classifiers.bayes.NaiveBayesMultinomial -t spam_train_1000.arff -T spam_test.arff
```

The spam classification dataset in the `q4/` directory was provided courtesy of Christian Shelton (cshelton@cs.ucr.edu). Each example corresponds to a particular email, and each feature correspondes to a particular word. For privacy reasons we have removed the actual words themselves from the data set, and instead label the features generically as `f1`, `f2`, etc. However, the data set is from a real spam classification task, so the results demonstrate the performance of these algorithms on a real-world problem. The `q4/` directory actually contains several different training files, named `spam_train_50.arff`, `spam_train_100.arff`, etc (the ".arff" format is the default format by WEKA), each containing the corresponding number of training examples. There is also a single test set `spam_test.arff`, which is a hold out set used for evaluating the classifier's performance.

(a) Run the `weka.classifiers.bayes.NaiveBayesMultinomial` classifier on the dataset and report the resulting error rates. Evaluate the performance of the classifier using each of the different training files (but each time using the same test file, `spam_test.arff`). Plot the error rate of the classifier versus the number of training examples.

(b) Repeat the previous part, but using the `weka.classifiers.functions.SMO` classifier, which implements the SMO algorithm to train an SVM. How does the performance of the SVM compare to that of Naive Bayes?

5. **Uniform convergence**

In class we proved that for any finite set of hypotheses $\mathcal{H} = \{h_1, \ldots, h_k\}$, if we pick the hypothesis $\hat{h}$ that minimizes the training error on a set of m examples, then with probability at least $(1-\delta)$,

$$\varepsilon(\hat{h}) \leq \left(\min_i \varepsilon(h_i)\right) + 2\sqrt{\frac{1}{2m}\log\frac{2k}{\delta}},$$

where $\varepsilon(h_i)$ is the generalization error of hypothesis h_i. Now consider a special case (often called the *realizable* case) where we know, a priori, that there is some hypothesis in our class $\mathcal{H}$ that achieves zero error on the distribution from which the data is drawn. Then we could obviously just use the above bound with $\min_i \varepsilon(h_i) = 0$; however, we can prove a better bound than this.

(a) Consider a learning algorithm which, after looking at m training examples, chooses some hypothesis $\hat{h} \in \mathcal{H}$ that makes zero mistakes on this training data. (By our assumption, there is at least one such hypothesis, possibly more.) Show that with probability $1-\delta$

$$\varepsilon(\hat{h}) \leq \frac{1}{m}\log\frac{k}{\delta}.$$

Notice that since we do not have a square root here, this bound is much tighter. [Hint: Consider the probability that a hypothesis with generalization error greater than γ makes no mistakes on the training data. Instead of the Hoeffding bound, you might also find the following inequality useful: $(1-\gamma)^m \leq e^{-\gamma m}$.]

(b) Rewrite the above bound as a sample complexity bound, i.e., in the form: for fixed δ and γ, for $\varepsilon(\hat{h}) \leq \gamma$ to hold with probability at least $(1 - \delta)$, it suffices that $m \geq f(k, \gamma, \delta)$ (i.e., $f(\cdot)$ is some function of k, γ, and δ).

CS 229, Public Course Problem Set #2 Solutions: Kernels, SVMs, and Theory

1. **Kernel ridge regression**

   In contrast to ordinary least squares which has a cost function

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

   we can also add a term that penalizes large weights in θ. In *ridge regression*, our least squares cost is regularized by adding a term $\lambda\|\theta\|^2$, where $\lambda > 0$ is a fixed (known) constant (regularization will be discussed at greater length in an upcoming course lecutre). The ridge regression cost function is then

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

   (a) Use the vector notation described in class to find a closed-form expreesion for the value of θ which minimizes the ridge regression cost function.

   Answer: Using the design matrix notation, we can rewrite $J(\theta)$ as

$$J(\theta) = \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y}) + \frac{\lambda}{2}\theta^T\theta.$$

   Then the gradient is

$$\nabla_\theta J(\theta) = X^T X\theta - X^T\vec{y} + \lambda\theta.$$

   Setting the gradient to 0 gives us

$$\begin{aligned} 0 &= X^T X\theta - X^T\vec{y} + \lambda\theta \\ \theta &= (X^T X + \lambda I)^{-1}X^T\vec{y}. \end{aligned}$$

   (b) Suppose that we want to use kernels to implicitly represent our feature vectors in a high-dimensional (possibly infinite dimensional) space. Using a feature mapping ϕ, the ridge regression cost function becomes

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(\theta^T \phi(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2}\|\theta\|^2.$$

   Making a prediction on a new input x_{new} would now be done by computing $\theta^T\phi(x_{\text{new}})$. Show how we can use the "kernel trick" to obtain a closed form for the prediction on the new input without ever explicitly computing $\phi(x_{\text{new}})$. You may assume that the parameter vector θ can be expressed as a linear combination of the input feature vectors; i.e., $\theta = \sum_{i=1}^{m}\alpha_i\phi(x^{(i)})$ for some set of parameters α_i.

[Hint: You may find the following identity useful:

$$(\lambda I + BA)^{-1}B = B(\lambda I + AB)^{-1}.$$

If you want, you can try to prove this as well, though this is not required for the problem.]

Answer: Let Φ be the design matrix associated with the feature vectors $\phi(x^{(i)})$. Then from parts (a) and (b),

$$\begin{aligned}\theta &= \left(\Phi^T\Phi + \lambda I\right)^{-1}\Phi^T\vec{y} \\ &= \Phi^T\left(\Phi\Phi^T + \lambda I\right)^{-1}\vec{y} \\ &= \Phi^T(K + \lambda I)^{-1}\vec{y}.\end{aligned}$$

where K is the kernel matrix for the training set (since $\Phi_{i,j} = \phi(x^{(i)})^T\phi(x^{(j)}) = K_{ij}$.) To predict a new value y_{new}, we can compute

$$\begin{aligned}\vec{y}_{\text{new}} &= \theta^T\phi(x_{\text{new}}) \\ &= \vec{y}^T(K + \lambda I)^{-1}\Phi\phi(x_{\text{new}}) \\ &= \sum_{i=1}^{m}\alpha_i K(x^{(i)}, x_{\text{new}}).\end{aligned}$$

where $\alpha = (K + \lambda I)^{-1}\vec{y}$. All these terms can be efficiently computing using the kernel function.

To prove the identity from the hint, we left-multiply by $\lambda(I + BA)$ and right-multiply by $\lambda(I + AB)$ on both sides. That is,

$$\begin{aligned}(\lambda I + BA)^{-1}B &= B(\lambda I + AB)^{-1} \\ B &= (\lambda I + BA)B(\lambda I + AB)^{-1} \\ B(\lambda I + AB) &= (\lambda I + BA)B \\ \lambda B + BAB &= \lambda B + BAB.\end{aligned}$$

This last line clearly holds, proving the identity.

2. **ℓ_2 norm soft margin SVMs**

   In class, we saw that if our data is not linearly separable, then we need to modify our support vector machine algorithm by introducing an error margin that must be minimized. Specifically, the formulation we have looked at is known as the ℓ_1 norm soft margin SVM. In this problem we will consider an alternative method, known as the ℓ_2 norm soft margin SVM. This new algorithm is given by the following optimization problem (notice that the slack penalties are now squared):

$$\begin{array}{ll}\min_{w,b,\xi} & \frac{1}{2}\|w\|^2 + \frac{C}{2}\sum_{i=1}^{m}\xi_i^2 \\ \text{s.t.} & y^{(i)}(w^Tx^{(i)} + b) \geq 1 - \xi_i,\ i = 1, \ldots, m\end{array}.$$

   (a) Notice that we have dropped the $\xi_i \geq 0$ constraint in the ℓ_2 problem. Show that these non-negativity constraints can be removed. That is, show that the optimal value of the objective will be the same whether or not these constraints are present.

   Answer: Consider a potential solution to the above problem with some $\xi < 0$. Then the constraint $y^{(i)}(w^Tx^{(i)} + b) \geq 1 - \xi_i$ would also be satisfied for $\xi_i = 0$, and the objective function would be lower, proving that this could not be an optimal solution.

(b) What is the Lagrangian of the ℓ_2 soft margin SVM optimization problem?
Answer:

$$\mathcal{L}(w,b,\xi,\alpha) = \frac{1}{2}w^T w + \frac{C}{2}\sum_{i=1}^m \xi_i^2 - \sum_{i=1}^m \alpha_i[y^{(i)}(w^T x^{(i)} + b) - 1 + \xi_i],$$

where $\alpha_i \geq 0$ for $i = 1, \ldots, m$.

(c) Minimize the Lagrangian with respect to w, b, and ξ by taking the following gradients: $\nabla_w \mathcal{L}$, $\frac{\partial \mathcal{L}}{\partial b}$, and $\nabla_\xi \mathcal{L}$, and then setting them equal to 0. Here, $\xi = [\xi_1, \xi_2, \ldots, \xi_m]^T$.
Answer: Taking the gradient with respect to w, we get

$$0 = \nabla_w \mathcal{L} = w - \sum_{i=1}^m \alpha_i y^{(i)} x^{(i)},$$

which gives us

$$w = \sum_{i=1}^m \alpha_i y^{(i)} x^{(i)}.$$

Taking the derivative with respect to b, we get

$$0 = \frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^m \alpha_i y^{(i)},$$

giving us

$$0 = \sum_{i=1}^m \alpha_i y^{(i)}.$$

Finally, taking the gradient with respect to ξ, we have

$$0 = \nabla_\xi \mathcal{L} = C\xi - \alpha,$$

where $\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_m]^T$. Thus, for each $i = 1, \ldots, m$, we get

$$0 = C\xi_i - \alpha_i \quad \Rightarrow \quad C\xi_i = \alpha_i.$$

(d) What is the dual of the ℓ_2 soft margin SVM optimization problem?

Answer: The objective function for the dual is

$$\begin{aligned} W(\alpha) &= \min_{w,b,\xi} \mathcal{L}(w,b,\xi,\alpha) \\ &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}(\alpha_i y^{(i)} x^{(i)})^T(\alpha_j y^{(j)} x^{(j)}) + \frac{1}{2}\sum_{i=1}^{m}\frac{\alpha_i}{\xi_i}\xi_i^2 \\ &\quad -\sum_{i=1}^{m}\alpha_i\left[y^{(i)}\left(\left(\sum_{j=1}^{m}\alpha_j y^{(j)} x^{(j)}\right)^T x^{(i)} + b\right) - 1 + \xi_i\right] \\ &= -\frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_i\alpha_j y^{(i)}y^{(j)}(x^{(i)})^T x^{(j)} + \frac{1}{2}\sum_{i=1}^{m}\alpha_i\xi_i \\ &\quad -\left(\sum_{i=1}^{m}\alpha_i y^{(i)}\right)b + \sum_{i=1}^{m}\alpha_i - \sum_{i=1}^{m}\alpha_i\xi_i \\ &= \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_i\alpha_j y^{(i)}y^{(j)}(x^{(i)})^T x^{(j)} - \frac{1}{2}\sum_{i=1}^{m}\alpha_i\xi_i \\ &= \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_i\alpha_j y^{(i)}y^{(j)}(x^{(i)})^T x^{(j)} - \frac{1}{2}\sum_{i=1}^{m}\frac{\alpha_i^2}{C}. \end{aligned}$$

Then the dual formulation of our problem is

$$\begin{array}{rl} \max_\alpha & \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i=1}^m\sum_{j=1}^m \alpha_i\alpha_j y^{(i)}y^{(j)}(x^{(i)})^T x^{(j)} - \frac{1}{2}\sum_{i=1}^m \frac{\alpha_i^2}{C} \\ \text{s.t.} & \alpha_i \geq 0,\ i = 1,\ldots,m \\ & \sum_{i=1}^m \alpha_i y^{(i)} = 0 \end{array}.$$

3. **SVM with Gaussian kernel**

   Consider the task of training a support vector machine using the Gaussian kernel $K(x,z) = \exp(-\|x-z\|^2/\tau^2)$. We will show that as long as there are no two identical points in the training set, we can always find a value for the bandwidth parameter τ such that the SVM achieves zero training error.

   (a) Recall from class that the decision function learned by the support vector machine can be written as

   $$f(x) = \sum_{i=1}^{m}\alpha_i y^{(i)} K(x^{(i)}, x) + b.$$

   Assume that the training data $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$ consists of points which are separated by at least a distance of ϵ; that is, $||x^{(j)} - x^{(i)}|| \geq \epsilon$ for any $i \neq j$. Find values for the set of parameters $\{\alpha_1, \ldots, \alpha_m, b\}$ and Gaussian kernel width τ such that $x^{(i)}$ is correctly classified, for all $i = 1, \ldots, m$. [Hint: Let $\alpha_i = 1$ for all i and $b = 0$. Now notice that for $y \in \{-1, +1\}$ the prediction on $x^{(i)}$ will be correct if $|f(x^{(i)}) - y^{(i)}| < 1$, so find a value of τ that satisfies this inequality for all i.]

Answer: First we set $\alpha_i = 1$ for all $i = 1, \ldots, m$ and $b = 0$. Then, for a training example $\{x^{(i)}, y^{(i)}\}$, we get

$$\begin{aligned}
\left|f(x^{(i)}) - y^{(i)}\right| &= \left|\sum_{j=1}^{m} y^{(j)} K(x^{(j)}, x^{(i)}) - y^{(i)}\right| \\
&= \left|\sum_{j=1}^{m} y^{(j)} \exp\left(-\|x^{(j)} - x^{(i)}\|^2/\tau^2\right) - y^{(i)}\right| \\
&= \left|y^{(i)} + \sum_{j\neq i} y^{(j)} \exp\left(\|x^{(j)} - x^{(i)}\|^2/\tau^2\right) - y^{(i)}\right| \\
&= \left|\sum_{j\neq i} y^{(j)} \exp\left(-\|x^{(j)} - x^{(i)}\|^2/\tau^2\right)\right| \\
&\leq \sum_{j\neq i} \left|y^{(j)} \exp\left(-\|x^{(j)} - x^{(i)}\|^2/\tau^2\right)\right| \\
&= \sum_{j\neq i} \left|y^{(j)}\right| \cdot \exp\left(\|x^{(j)} - x^{(i)}\|^2/\tau^2\right) \\
&= \sum_{j\neq i} \exp\left(-\|x^{(j)} - x^{(i)}\|^2/\tau^2\right) \\
&\leq \sum_{j\neq i} \exp\left(-\epsilon^2/\tau^2\right) \\
&= (m-1)\exp\left(-\epsilon^2/\tau^2\right).
\end{aligned}$$

The first inequality comes from repeated application of the triangle inequality $|a + b| \leq |a| + |b|$, and the second inequality (1) from the assumption that $||x^{(j)} - x^{(i)}|| \geq \epsilon$ for all $i \neq j$. Thus we need to choose a γ such that

$$(m-1)\exp(-\epsilon^2/\tau^2) < 1,$$

or

$$\tau < \frac{\epsilon}{\log(m-1)}.$$

By choosing, for example, $\tau = \epsilon/\log m$ we are done.

(b) Suppose we run a SVM with slack variables using the parameter τ you found in part (a). Will the resulting classifier necessarily obtain zero training error? Why or why not? A short explanation (without proof) will suffice.

Answer: The classifier will obtain zero training error. The SVM without slack variables will always return zero training error if it is able to find a solution, so all that remains to be shown is that there exists at least one feasible point.

Consider the constraint $y^{(i)}(w^T x^{(i)} + b)$ for some i, and let $b = 0$. Then

$$y^{(i)}(w^T x^{(i)} + b) = y^{(i)} \cdot f(x^{(i)}) > 0$$

since $f(x^{(i)})$ and $y^{(i)}$ have the same sign, and shown above. Therefore, as we choose all the α_i's large enough, $y^{(i)}(w^T x^{(i)} + b) > 1$, so the optimization problem is feasible.

(c) Suppose we run the SMO algorithm to train an SVM with slack variables, under the conditions stated above, using the value of τ you picked in the previous part, and using some arbitrary value of C (which you do not know beforehand). Will this necessarily result in a classifier that achieve zero training error? Why or why not? Again, a short explanation is sufficient.

Answer: The resulting classifier will not necessarily obtain zero training error. The C parameter controls the relative weights of the $(C\sum_{i=1}^{m}\xi_i)$ and $(\frac{1}{2}||w||^2)$ terms of the SVM training objective. If the C parameter is sufficiently small, then the former component will have relatively little contribution to the objective. In this case, a weight vector which has a very small norm but does not achieve zero training error may achieve a lower objective value than one which achieves zero training error. For example, you can consider the extreme case where $C = 0$, and the objective is just the norm of w. In this case, $w = 0$ is the solution to the optimization problem regardless of the choise of τ, this this may not obtain zero training error.

4. **Naive Bayes and SVMs for Spam Classification**

In this question you'll look into the Naive Bayes and Support Vector Machine algorithms for a spam classification problem. However, instead of implementing the algorithms yourself, you'll use a freely available machine learning library. There are many such libraries available, with different strengths and weaknesses, but for this problem you'll use the WEKA machine learning package, available at `http://www.cs.waikato.ac.nz/ml/weka/`. WEKA implements many standard machine learning algorithms, is written in Java, and has both a GUI and a command line interface. It is not the best library for very large-scale data sets, but it is very nice for playing around with many different algorithms on medium size problems.

You can download and install WEKA by following the instructions given on the website above. To use it from the command line, you first need to install a java runtime environment, then add the `weka.jar` file to your `CLASSPATH` environment variable. Finally, you can call WEKA using the command:

```
java <classifier> -t <training file> -T <test file>
```

For example, to run the Naive Bayes classifier (using the multinomial event model) on our provided spam data set by running the command:

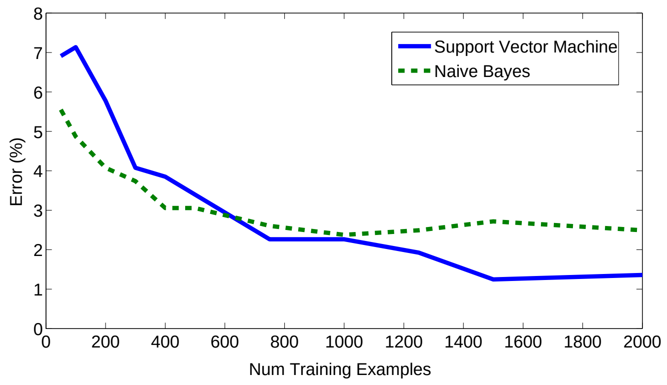
```
java weka.classifiers.bayes.NaiveBayesMultinomial -t spam_train_1000.arff -T spam_test.arff
```

The spam classification dataset in the `q4/` directory was provided courtesy of Christian Shelton (cshelton@cs.ucr.edu). Each example corresponds to a particular email, and each feature correspondes to a particular word. For privacy reasons we have removed the actual words themselves from the data set, and instead label the features generically as `f1`, `f2`, etc. However, the data set is from a real spam classification task, so the results demonstrate the performance of these algorithms on a real-world problem. The `q4/` directory actually contains several different training files, named `spam_train_50.arff`, `spam_train_100.arff`, etc (the ".arff" format is the default format by WEKA), each containing the corresponding number of training examples. There is also a single test set `spam_test.arff`, which is a hold out set used for evaluating the classifier's performance.

(a) Run the `weka.classifiers.bayes.NaiveBayesMultinomial` classifier on the dataset and report the resulting error rates. Evaluate the performance of the classifier using each of the different training files (but each time using the same test file, `spam_test.arff`). Plot the error rate of the classifier versus the number of training examples.

(b) Repeat the previous part, but using the `weka.classifiers.functions.SMO` classifier, which implements the SMO algorithm to train an SVM. How does the performance of the SVM compare to that of Naive Bayes?

Answer: Using the above command line arguments to run the classifier, we obtain the following error rates for the two algorithms:



For small amounts of data, Naive Bayes performs better than the Support Vector Machine. However, as the amount of data grows, the SVM achieves a better error rate.

5. **Uniform convergence**

In class we proved that for any finite set of hypotheses $\mathcal{H} = \{h_1, \ldots, h_k\}$, if we pick the hypothesis $\hat{h}$ that minimizes the training error on a set of m examples, then with probability at least $(1 - \delta)$,

$$\varepsilon(\hat{h}) \leq \left(\min_i \varepsilon(h_i)\right) + 2\sqrt{\frac{1}{2m}\log\frac{2k}{\delta}},$$

where $\varepsilon(h_i)$ is the generalization error of hypothesis h_i. Now consider a special case (often called the *realizable* case) where we know, a priori, that there is some hypothesis in our class $\mathcal{H}$ that achieves zero error on the distribution from which the data is drawn. Then we could obviously just use the above bound with $\min_i \varepsilon(h_i) = 0$; however, we can prove a better bound than this.

(a) Consider a learning algorithm which, after looking at m training examples, chooses some hypothesis $\hat{h} \in \mathcal{H}$ that makes zero mistakes on this training data. (By our assumption, there is at least one such hypothesis, possibly more.) Show that with probability $1 - \delta$

$$\varepsilon(\hat{h}) \leq \frac{1}{m}\log\frac{k}{\delta}.$$

Notice that since we do not have a square root here, this bound is much tighter. [Hint: Consider the probability that a hypothesis with generalization error greater than γ makes no mistakes on the training data. Instead of the Hoeffding bound, you might also find the following inequality useful: $(1 - \gamma)^m \leq e^{-\gamma m}$.]

Answer: Let $h \in \mathcal{H}$ be a hypothesis with true error greater than γ. Then

$$P(\text{“}h\text{ predicts correctly”}) \leq 1 - \gamma,$$

so

$$P(\text{“}h \text{ predicts correctly } m \text{ times”}) \leq (1-\gamma)^m \leq e^{-\gamma m}.$$

Applying the union bound,

$$P(\exists h \in \mathcal{H}, \text{ s.t. } \varepsilon(h) > \gamma \text{ and “h predicts correct } m \text{ times”}) \leq k e^{-\gamma m}.$$

We want to make this probability equal to δ, so we set

$$k e^{-\gamma m} = \delta,$$

which gives us

$$\gamma = \frac{1}{m} \log \frac{k}{\delta}.$$

This impiles that with probability $1 - \delta$,

$$\varepsilon(\hat{h}) \leq \frac{1}{m} \log \frac{k}{\delta}.$$

(b) Rewrite the above bound as a sample complexity bound, i.e., in the form: for fixed δ and γ, for $\varepsilon(\hat{h}) \leq \gamma$ to hold with probability at least $(1-\delta)$, it suffices that $m \geq f(k, \gamma, \delta)$ (i.e., $f(\cdot)$ is some function of k, γ, and δ).

Answer: From part (a), if we take the equation,

$$k e^{-\gamma m} = \delta$$

and solve for m, we obtain

$$m = \frac{1}{\gamma} \log \frac{k}{\delta}.$$

Therefore, for m larger than this, $\varepsilon(\hat{h}) \leq \gamma$ will hold with probability at least $1 - \delta$.

CS 229, Public Course
Problem Set #3: Learning Theory and Unsupervised Learning

1. **Uniform convergence and Model Selection**

   In this problem, we will prove a bound on the error of a simple model selection procedure.

   Let there be a binary classification problem with labels $y \in \{0,1\}$, and let $\mathcal{H}_1 \subseteq \mathcal{H}_2 \subseteq \ldots \subseteq \mathcal{H}_k$ be k different finite hypothesis classes ($|\mathcal{H}_i| < \infty$). Given a dataset S of m iid training examples, we will divide it into a training set S_{train} consisting of the first $(1-\beta)m$ examples, and a hold-out cross validation set S_{cv} consisting of the remaining βm examples. Here, $\beta \in (0,1)$.

   Let $\hat{h}_i = \arg\min_{h\in\mathcal{H}_i} \hat{\varepsilon}_{S_{\text{train}}}(h)$ be the hypothesis in $\mathcal{H}_i$ with the lowest *training* error (on S_{train}). Thus, $\hat{h}_i$ would be the hypothesis returned by training (with empirical risk minimization) using hypothesis class $\mathcal{H}_i$ and dataset S_{train}. Also let $h_i^\star = \arg\min_{h\in\mathcal{H}_i} \varepsilon(h)$ be the hypothesis in $\mathcal{H}_i$ with the lowest *generalization* error.

   Suppose that our algorithm first finds all the $\hat{h}_i$'s using empirical risk minimization then uses the hold-out cross validation set to select a hypothesis from this the $\{\hat{h}_1, \ldots, \hat{h}_k\}$ with minimum training error. That is, the algorithm will output

   $$\hat{h} = \arg\min_{h\in\{\hat{h}_1,\ldots,\hat{h}_k\}} \hat{\varepsilon}_{S_{\text{cv}}}(h).$$

   For this question you will prove the following bound. Let any $\delta > 0$ be fixed. Then with probability at least $1-\delta$, we have that

   $$\varepsilon(\hat{h}) \le \min_{i=1,\ldots,k}\left(\varepsilon(h_i^*) + \sqrt{\frac{2}{(1-\beta)m}\log\frac{4|\mathcal{H}_i|}{\delta}}\right) + \sqrt{\frac{2}{2\beta m}\log\frac{4k}{\delta}}$$

   (a) Prove that with probability at least $1-\frac{\delta}{2}$, for all $\hat{h}_i$,

   $$|\varepsilon(\hat{h}_i) - \hat{\varepsilon}_{S_{\text{cv}}}(\hat{h}_i)| \le \sqrt{\frac{1}{2\beta m}\log\frac{4k}{\delta}}.$$

   (b) Use part (a) to show that with probability $1-\frac{\delta}{2}$,

   $$\varepsilon(\hat{h}) \le \min_{i=1,\ldots,k} \varepsilon(\hat{h}_i) + \sqrt{\frac{2}{\beta m}\log\frac{4k}{\delta}}.$$

   (c) Let $j = \arg\min_i \varepsilon(\hat{h}_i)$. We know from class that for $\mathcal{H}_j$, with probability $1-\frac{\delta}{2}$

   $$|\varepsilon(\hat{h}_j) - \hat{\varepsilon}_{S_{\text{train}}}(h_j^\star)| \le \sqrt{\frac{2}{(1-\beta)m}\log\frac{4|\mathcal{H}_j|}{\delta}}, \ \ \forall h_j \in \mathcal{H}_j.$$

   Use this to prove the final bound given at the beginning of this problem.

2. **VC Dimension**

   Let the input domain of a learning problem be $\mathcal{X} = \mathbb{R}$. Give the VC dimension for each of the following classes of hypotheses. In each case, if you claim that the VC dimension is d, then you need to show that the hypothesis class can shatter d points, and explain why there are no $d+1$ points it can shatter.

   - $h(x) = \mathbf{1}\{a < x\}$, with parameter $a \in \mathbb{R}$.
   - $h(x) = \mathbf{1}\{a < x < b\}$, with parameters $a, b \in \mathbb{R}$.
   - $h(x) = \mathbf{1}\{a \sin x > 0\}$, with parameter $a \in \mathbb{R}$.
   - $h(x) = \mathbf{1}\{\sin(x + a) > 0\}$, with parameter $a \in \mathbb{R}$.

3. **ℓ_1 regularization for least squares**

   In the previous problem set, we looked at the least squares problem where the objective function is augmented with an additional regularization term $\lambda\|\theta\|_2^2$. In this problem we'll consider a similar regularized objective but this time with a penalty on the ℓ_1 norm of the parameters $\lambda\|\theta\|_1$, where $\|\theta\|_1$ is defined as $\sum_i |\theta_i|$. That is, we want to minimize the objective

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})^2 + \lambda\sum_{i=1}^{n}|\theta_i|.$$

   There has been a great deal of recent interest in ℓ_1 regularization, which, as we will see, has the benefit of outputting sparse solutions (i.e., many components of the resulting θ are equal to zero).

   The ℓ_1 regularized least squares problem is more difficult than the unregularized or ℓ_2 regularized case, because the ℓ_1 term is not differentiable. However, there have been many efficient algorithms developed for this problem that work very well in practive. One very straightforward approach, which we have already seen in class, is the coordinate descent method. In this problem you'll derive and implement a coordinate descent algorithm for ℓ_1 regularized least squares, and apply it to test data.

   (a) Here we'll derive the coordinate descent update for a given θ_i. Given the X and $\vec{y}$ matrices, as defined in the class notes, as well a parameter vector θ, how can we adjust θ_i so as to minimize the optimization objective? To answer this question, we'll rewrite the optimization objective above as

$$J(\theta) = \frac{1}{2}\|X\theta - \vec{y}\|_2^2 + \lambda\|\theta\|_1 = \frac{1}{2}\|X\bar{\theta} + X_i\theta_i - \vec{y}\|_2^2 + \lambda\|\bar{\theta}\|_1 + \lambda|\theta_i|$$

   where $X_i \in \mathbb{R}^m$ denotes the ith column of X, and $\bar{\theta}$ is equal to θ except with $\bar{\theta}_i = 0$; all we have done in rewriting the above expression is to make the θ_i term explicit in the objective. However, this still contains the $|\theta_i|$ term, which is non-differentiable and therefore difficult to optimize. To get around this we make the observation that the sign of θ_i must either be non-negative or non-positive. But if we *knew* the sign of θ_i, then $|\theta_i|$ becomes just a linear term. That, is, we can rewrite the objective as

$$J(\theta) = \frac{1}{2}\|X\bar{\theta} + X_i\theta_i - \vec{y}\|_2^2 + \lambda\|\bar{\theta}\|_1 + \lambda s_i\theta_i$$

   where s_i denotes the sign of θ_i, $s_i \in \{-1, 1\}$. In order to update θ_i, we can just compute the optimal θ_i for both possible values of s_i (making sure that we restrict the optimal θ_i to obey the sign restriction we used to solve for it), then look to see which achieves the best objective value.

For each of the possible values of s_i, compute the resulting optimal value of θ_i. [Hint: to do this, you can fix s_i in the above equation, then differentiate with respect to θ_i to find the best value. Finally, clip θ_i so that it lies in the allowable range — i.e., for $s_i = 1$, you need to clip θ_i such that $\theta_i \geq 0$.]

(b) Implement the above coordinate descent algorithm using the updates you found in the previous part. We have provided a skeleton `theta = l1ls(X,y,lambda)` function in the `q3/` directory. To implement the coordinate descent algorithm, you should repeatedly iterate over all the θ_i's, adjusting each as you found above. You can terminate the process when θ changes by less than 10^-5 after all n of the updates.

(c) Test your implementation on the data provided in the `q3/` directory. The `[X, y, theta_true] = load_data;` function will load all the data — the data was generated by `y = X*theta_true + 0.05*randn(20,1)`, but `theta_true` is sparse, so that very few of the columns of `X` actually contain relevant features. Run your `l1ls.m` implementation on this data set, ranging λ from 0.001 to 10. Comment briefly on how this algorithm might be used for feature selection.

4. **K-Means Clustering**

In this problem you'll implement the K-means clustering algorithm on a synthetic data set. There is code and data for this problem in the `q4/` directory. Run `load 'X.dat';` to load the data file for clustering. Implement the `[clusters, centers] = k_means(X, k)` function in this directory. As input, this function takes the $m \times n$ data matrix `X` and the number of clusters `k`. It should output a m element vector, `clusters`, which indicates which of the clusters each data point belongs to, and a $k \times n$ matrix, `centers`, which contains the centroids of each cluster. Run the algorithm on the data provided, with $k = 3$ and $k = 4$. Plot the cluster assignments and centroids for each iteration of the algorithm using the `draw_clusters(X, clusters, centroids)` function. For each k, be sure to run the algorithm several times using different initial centroids.

5. **The Generalized EM algorithm**

When attempting to run the EM algorithm, it may sometimes be difficult to perform the M step exactly — recall that we often need to implement numerical optimization to perform the maximization, which can be costly. Therefore, instead of finding the global maximum of our lower bound on the log-likelihood, and alternative is to just increase this lower bound a little bit, by taking one step of gradient ascent, for example. This is commonly known as the Generalized EM (GEM) algorithm.

Put slightly more formally, recall that the M-step of the standard EM algorithm performs the maximization

$$\theta := \arg\max_\theta \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$$

The GEM algorithm, in constrast, performs the following update in the M-step:

$$\theta := \theta + \alpha \nabla_\theta \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}$$

where α is a learning rate which we assume is choosen small enough such that we do not decrease the objective function when taking this gradient step.

(a) Prove that the GEM algorithm described above converges. To do this, you should show that the the likelihood is monotonically improving, as it does for the EM algorithm — i.e., show that $\ell(\theta^{(t+1)}) \geq \ell(\theta^{(t)})$.

(b) Instead of using the EM algorithm at all, suppose we just want to apply gradient ascent to maximize the log-likelihood directly. In other words, we are trying to maximize the (non-convex) function

$$\ell(\theta) = \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta)$$

so we could simply use the update

$$\theta := \theta + \alpha \nabla_\theta \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta).$$

Show that this procedure in fact gives the same update as the GEM algorithm described above.

CS 229, Public Course
Problem Set #3 Solutions: Learning Theory and Unsupervised Learning

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1. **Uniform convergence and Model Selection**

   In this problem, we will prove a bound on the error of a simple model selection procedure.

   Let there be a binary classification problem with labels $y \in \{0, 1\}$, and let $\mathcal{H}_1 \subseteq \mathcal{H}_2 \subseteq \ldots \subseteq \mathcal{H}_k$ be k different finite hypothesis classes ($|\mathcal{H}_i| < \infty$). Given a dataset S of m iid training examples, we will divide it into a training set S_{train} consisting of the first $(1-\beta)m$ examples, and a hold-out cross validation set S_{cv} consisting of the remaining βm examples. Here, $\beta \in (0, 1)$.

   Let $\hat{h}_i = \arg\min_{h \in \mathcal{H}_i} \hat{\varepsilon}_{S_{\text{train}}}(h)$ be the hypothesis in $\mathcal{H}_i$ with the lowest *training* error (on S_{train}). Thus, $\hat{h}_i$ would be the hypothesis returned by training (with empirical risk minimization) using hypothesis class $\mathcal{H}_i$ and dataset S_{train}. Also let $h_i^\star = \arg\min_{h \in \mathcal{H}_i} \varepsilon(h)$ be the hypothesis in $\mathcal{H}_i$ with the lowest *generalization* error.

   Suppose that our algorithm first finds all the $\hat{h}_i$'s using empirical risk minimization then uses the hold-out cross validation set to select a hypothesis from this the $\{\hat{h}_1, \ldots, \hat{h}_k\}$ with minimum training error. That is, the algorithm will output

$$\hat{h} = \arg \min_{h \in \{\hat{h}_1, \ldots, \hat{h}_k\}} \hat{\varepsilon}_{S_{\text{cv}}}(h).$$

   For this question you will prove the following bound. Let any $\delta > 0$ be fixed. Then with probability at least $1 - \delta$, we have that

$$\varepsilon(\hat{h}) \leq \min_{i=1,\ldots,k} \left(\varepsilon(h_i^*) + \sqrt{\frac{2}{(1-\beta)m} \log \frac{4|\mathcal{H}_i|}{\delta}} \right) + \sqrt{\frac{2}{2\beta m} \log \frac{4k}{\delta}}$$

   (a) Prove that with probability at least $1 - \frac{\delta}{2}$, for all $\hat{h}_i$,

$$|\varepsilon(\hat{h}_i) - \hat{\varepsilon}_{S_{\text{cv}}}(\hat{h}_i)| \leq \sqrt{\frac{1}{2\beta m} \log \frac{4k}{\delta}}.$$

   Answer: For each $\hat{h}_i$, the empirical error on the cross-validation set, $\hat{\varepsilon}(\hat{h}_i)$ represents the average of βm random variables with mean $\varepsilon(\hat{h}_i)$, so by the Hoeffding inequality for any $\hat{h}_i$,

$$P(|\varepsilon(\hat{h}_i) - \hat{\varepsilon}_{S_{\text{cv}}}(\hat{h}_i)| \geq \gamma) \leq 2\exp(-2\gamma^2 \beta m).$$

   As in the class notes, to insure that this holds for all $\hat{h}_i$, we need to take the union over all k of the $\hat{h}_i$'s.

$$P(\exists i, s.t. |\varepsilon(\hat{h}_i) - \hat{\varepsilon}_{S_{\text{cv}}}(\hat{h}_i)| \geq \gamma) \leq 2k\exp(-2\gamma^2 \beta m).$$

Setting this term equal to $\delta/2$ and solving for γ yields

$$\gamma = \sqrt{\frac{1}{2\beta m} \log \frac{4k}{\delta}}$$

proving the desired bound.

(b) Use part (a) to show that with probability $1 - \frac{\delta}{2}$,

$$\varepsilon(\hat{h}) \leq \min_{i=1,\ldots,k} \varepsilon(\hat{h}_i) + \sqrt{\frac{2}{\beta m} \log \frac{4k}{\delta}}.$$

Answer: Let $j = \arg\min_i \varepsilon(\hat{h}_i)$. Using part (a), with probability at least $1 - \frac{\delta}{2}$

$$\begin{aligned}
\varepsilon(\hat{h}) &\leq \hat{\varepsilon}_{S_{\rm cv}}(\hat{h}) + \sqrt{\frac{1}{2\beta m} \log \frac{4k}{\delta}} \\
&= \min_i \hat{\varepsilon}_{S_{\rm cv}}(\hat{h}_i) + \sqrt{\frac{1}{2\beta m} \log \frac{4k}{\delta}} \\
&\leq \hat{\varepsilon}_{S_{\rm cv}}(\hat{h}_j) + \sqrt{\frac{1}{2\beta m} \log \frac{4k}{\delta}} \\
&\leq \varepsilon(\hat{h}_j) + 2\sqrt{\frac{1}{2\beta m} \log \frac{4k}{\delta}} \\
&= \min_{i=1,\ldots,k} \varepsilon(\hat{h}_i) + \sqrt{\frac{2}{\beta m} \log \frac{4k}{\delta}}
\end{aligned}$$

(c) Let $j = \arg\min_i \varepsilon(\hat{h}_i)$. We know from class that for $\mathcal{H}_j$, with probability $1 - \frac{\delta}{2}$

$$|\varepsilon(\hat{h}_j) - \hat{\varepsilon}_{S_{\rm train}}(h_j^\star)| \leq \sqrt{\frac{2}{(1-\beta)m} \log \frac{4|\mathcal{H}_j|}{\delta}}, \quad \forall h_j \in \mathcal{H}_j.$$

Use this to prove the final bound given at the beginning of this problem.

Answer: The bounds in parts (a) and (c) both hold simultaneously with probability $(1 - \frac{\delta}{2})^2 = 1 - \delta + \frac{\delta^2}{4} > 1 - \delta$, so with probablity greater than $1 - \delta$,

$$\varepsilon(\hat{h}) \leq \varepsilon(h_j^\star) + 2\sqrt{\frac{1}{2(1-\gamma)m} \log \frac{2|\mathcal{H}_j|}{\frac{\delta}{2}}} + 2\sqrt{\frac{1}{2\gamma m} \log \frac{2k}{\frac{\delta}{2}}}$$

which is equivalent to the bound we want to show.

2. **VC Dimension**

Let the input domain of a learning problem be $\mathcal{X} = \mathbb{R}$. Give the VC dimension for each of the following classes of hypotheses. In each case, if you claim that the VC dimension is d, then you need to show that the hypothesis class can shatter d points, and explain why there are no $d + 1$ points it can shatter.

- $h(x) = \mathbf{1}\{a < x\}$, with parameter $a \in \mathbb{R}$.

  Answer: VC-dimension = 1.

  (a) It can shatter point $\{0\}$, by choosing a to be 2 and -2.

  (b) It cannot shatter any two points $\{x_1, x_2\}$, $x_1 < x_2$, because the labelling $x_1 = 1$ and $x_2 = 0$ cannot be realized.

- $h(x) = \mathbf{1}\{a < x < b\}$, with parameters $a, b \in \mathbb{R}$.

  Answer: VC-dimension = 2.

  (a) It can shatter points $\{0, 2\}$ by choosing (a, b) to be $(3, 5)$, $(-1, 1)$, $(1, 3)$, $(-1, 3)$.

  (b) It cannot shatter any three points $\{x_1, x_2, x_3\}$, $x_1 < x_2 < x_3$, because the labelling $x_1 = x_3 = 1$, $x_2 = 0$ cannot be realized.

- $h(x) = \mathbf{1}\{a \sin x > 0\}$, with parameter $a \in \mathbb{R}$.

  Answer: VC-dimension = 1. a controls the *amplitude* of the sine curve.

  (a) It can shatter point $\{\frac{\pi}{2}\}$ by choosing a to be 1 and -1.

  (b) It cannot shatter any two points $\{x_1, x_2\}$, since, the labellings of x_1 and x_2 will flip together. If $x_1 = x_2 = 1$ for some a, then we cannot achieve $x_1 \neq x_2$. If $x_1 \neq x_2$ for some a, then we cannot achieve $x_1 = x_2 = 1$ ($x_1 = x_2 = 0$ can be achieved by setting $a = 0$).

- $h(x) = \mathbf{1}\{\sin(x + a) > 0\}$, with parameter $a \in \mathbb{R}$.

  Answer: VC-dimension = 2. a controls the *phase* of the sine curve.

  (a) It can shatter points $\{\frac{\pi}{4}, \frac{3\pi}{4}\}$, by choosing a to be 0, $\frac{\pi}{2}$, π, and $\frac{3\pi}{2}$.

  (b) It cannot shatter any three points $\{x_1, x_2, x_3\}$. Since sine has a preiod of 2π, let's define $x'_i = x_i \mod 2\pi$. W.l.o.g., assume $x'_1 < x'_2 < x'_3$. If the labelling of $x_1 = x_2 = x_3 = 1$ can be realized, then the labelling of $x_1 = x_3 = 1$, $x_2 = 0$ will not be realizable. Notice the similarity to the second question.

3. **ℓ_1 regularization for least squares**

   In the previous problem set, we looked at the least squares problem where the objective function is augmented with an additional regularization term $\lambda\|\theta\|_2^2$. In this problem we'll consider a similar regularized objective but this time with a penalty on the ℓ_1 norm of the parameters $\lambda\|\theta\|_1$, where $\|\theta\|_1$ is defined as $\sum_i |\theta_i|$. That is, we want to minimize the objective

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})^2 + \lambda\sum_{i=1}^{n}|\theta_i|.$$

   There has been a great deal of recent interest in ℓ_1 regularization, which, as we will see, has the benefit of outputting sparse solutions (i.e., many components of the resulting θ are equal to zero).

   The ℓ_1 regularized least squares problem is more difficult than the unregularized or ℓ_2 regularized case, because the ℓ_1 term is not differentiable. However, there have been many efficient algorithms developed for this problem that work very well in practive. One very straightforward approach, which we have already seen in class, is the coordinate descent method. In this problem you'll derive and implement a coordinate descent algorithm for ℓ_1 regularized least squares, and apply it to test data.

(a) Here we'll derive the coordinate descent update for a given θ_i. Given the X and $\vec{y}$ matrices, as defined in the class notes, as well a parameter vector θ, how can we adjust θ_i so as to minimize the optimization objective? To answer this question, we'll rewrite the optimization objective above as

$$J(\theta) = \frac{1}{2}\|X\theta - \vec{y}\|_2^2 + \lambda\|\theta\|_1 = \frac{1}{2}\|X\bar{\theta} + X_i\theta_i - \vec{y}\|_2^2 + \lambda\|\bar{\theta}\|_1 + \lambda|\theta_i|$$

where $X_i \in \mathbb{R}^m$ denotes the ith column of X, and $\bar{\theta}$ is equal to θ except with $\bar{\theta}_i = 0$; all we have done in rewriting the above expression is to make the θ_i term explicit in the objective. However, this still contains the $|\theta_i|$ term, which is non-differentiable and therefore difficult to optimize. To get around this we make the observation that the sign of θ_i must either be non-negative or non-positive. But if we *knew* the sign of θ_i, then $|\theta_i|$ becomes just a linear term. That, is, we can rewrite the objective as

$$J(\theta) = \frac{1}{2}\|X\bar{\theta} + X_i\theta_i - \vec{y}\|_2^2 + \lambda\|\bar{\theta}\|_1 + \lambda s_i\theta_i$$

where s_i denotes the sign of θ_i, $s_i \in \{-1, 1\}$. In order to update θ_i, we can just compute the optimal θ_i for both possible values of s_i (making sure that we restrict the optimal θ_i to obey the sign restriction we used to solve for it), then look to see which achieves the best objective value.

For each of the possible values of s_i, compute the resulting optimal value of θ_i. [Hint: to do this, you can fix s_i in the above equation, then differentiate with respect to θ_i to find the best value. Finally, clip θ_i so that it lies in the allowable range — i.e., for $s_i = 1$, you need to clip θ_i such that $\theta_i \geq 0$.]

Answer: For $s_i = 1$,

$$\begin{aligned} J(\theta) &= \frac{1}{2}\mathrm{tr}(X\bar{\theta} + X_i\theta_i - \vec{y})^T(X\bar{\theta} + X_i\theta_i - \vec{y}) + \lambda\|\bar{\theta}\|_1 + \lambda\theta_i \\ &= \frac{1}{2}\left(X_i^TX_i\theta_i^2 + 2X_i^T(X\bar{\theta} - \vec{y})\theta_i + \|X\bar{\theta} - \vec{y}\|_2^2\right) + \lambda\|\bar{\theta}\|_1 + \lambda\theta_i, \end{aligned}$$

so

$$\frac{\partial J(\theta)}{\partial\theta_i} = X_i^TX_i\theta + X_i^T(X\bar{\theta} - \vec{y}) + \lambda$$

which means the optimal θ_i is given by

$$\theta_i = \max\left\{\frac{-X_i^T(X\bar{\theta} - \vec{y}) - \lambda}{X_i^TX_i}, 0\right\}.$$

Similarly, for $s_i = -1$, the optimal θ_i is given by

$$\theta_i = \min\left\{\frac{-X_i^T(X\bar{\theta} - \vec{y}) + \lambda}{X_i^TX_i}, 0\right\}.$$

(b) Implement the above coordinate descent algorithm using the updates you found in the previous part. We have provided a skeleton `theta = l1ls(X,y,lambda)` function in the `q3/` directory. To implement the coordinate descent algorithm, you should repeatedly iterate over all the θ_i's, adjusting each as you found above. You can terminate the process when θ changes by less than 10^-5 after all n of the updates.

Answer: The following is our implementation of `l1ls.m`:

```
function theta = l1l2(X,y,lambda)

m = size(X,1);
n = size(X,2);
theta = zeros(n,1);
old_theta = ones(n,1);

while (norm(theta - old_theta) > 1e-5)
  old_theta = theta;
  for i=1:n,
    % compute possible values for theta
    theta(i) = 0;
    theta_i(1) = max((-X(:,i)'*(X*theta - y) - lambda) / (X(:,i)'*X(:,i)), 0);
    theta_i(2) = min((-X(:,i)'*(X*theta - y) + lambda) / (X(:,i)'*X(:,i)), 0);

    % get objective value for both possible thetas
    theta(i) = theta_i(1);
    obj_theta(1) = 0.5*norm(X*theta - y)^2 + lambda*norm(theta,1);
    theta(i) = theta_i(2);
    obj_theta(2) = 0.5*norm(X*theta - y)^2 + lambda*norm(theta,1);

    % pick the theta which minimizes the objective
    [min_obj, min_ind] = min(obj_theta);
    theta(i) = theta_i(min_ind);
  end
end
```

(c) Test your implementation on the data provided in the `q3/` directory. The `[X, y, theta_true] = load_data;` function will load all the data — the data was generated by `y = X*theta_true + 0.05*randn(20,1)`, but `theta_true` is sparse, so that very few of the columns of `X` actually contain relevant features. Run your `l1ls.m` implementation on this data set, ranging λ from 0.001 to 10. Comment briefly on how this algorithm might be used for feature selection.

Answer: For $\lambda = 1$, our implementation of l_1 regularized least squares recovers the exact sparsity pattern of the true parameter that generated the data. In constrast, using any amount of l_2 regularization still leads to θ's that contain no zeros. This suggests that the l_1 regularization could be very useful as a feature selection algorithm: we could run l_1 regularized least squares to see which coefficients are non-zero, then select only these features for use with either least-squares or possibly a completely different machine learning algorithm.

4. **K-Means Clustering**

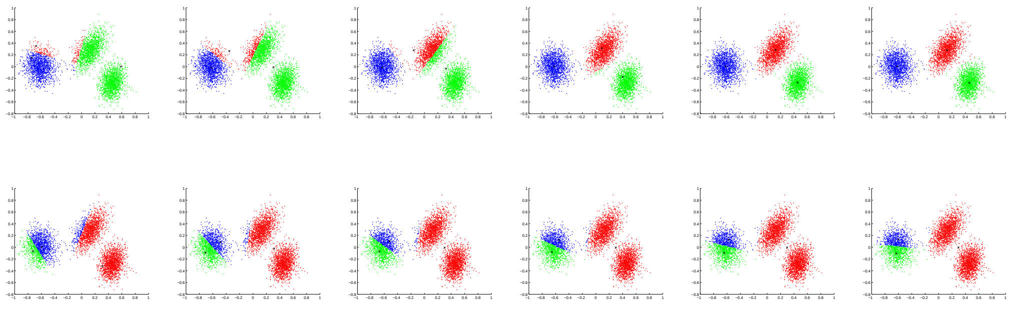
In this problem you'll implement the K-means clustering algorithm on a synthetic data set. There is code and data for this problem in the `q4/` directory. Run `load 'X.dat';` to load the data file for clustering. Implement the `[clusters, centers] = k_means(X, k)` function in this directory. As input, this function takes the $m \times n$ data matrix `X` and the number of clusters `k`. It should output a m element vector, `clusters`, which indicates which of the clusters each data point belongs to, and a $k \times n$ matrix, `centers`, which contains the centroids of each cluster. Run the algorithm on the data provided, with $k = 3$

and $k = 4$. Plot the cluster assignments and centroids for each iteration of the algorithm using the `draw_clusters(X, clusters, centroids)` function. For each k, be sure to run the algorithm several times using different initial centroids.

Answer: The following is our implementation of `k_means.m`:

```
function [clusters, centroids] = k_means(X, k)

m = size(X,1);
n = size(X,2);
oldcentroids = zeros(k,n);
centroids = X(ceil(rand(k,1)*m),:);

while (norm(oldcentroids - centroids) > 1e-15)
  oldcentroids = centroids;
  % compute cluster assignments
  for i=1:m,
    dists = sum((repmat(X(i,:), k, 1) - centroids).^2, 2);
    [min_dist, clusters(i,1)] = min(dists);
  end

  draw_clusters(X, clusters, centroids);
  pause(0.1);

  % compute cluster centroids
  for i=1:k,
    centroids(i,:) = mean(X(clusters == i, :));
  end
end
```

Below we show the centroid evolution for two typical runs with $k = 3$. Note that the different starting positions of the clusters lead to do different final clusterings.



5. **The Generalized EM algorithm**

When attempting to run the EM algorithm, it may sometimes be difficult to perform the M step exactly — recall that we often need to implement numerical optimization to perform the maximization, which can be costly. Therefore, instead of finding the global maximum of our lower bound on the log-likelihood, and alternative is to just increase this lower bound a little bit, by taking one step of gradient ascent, for example. This is commonly known as the Generalized EM (GEM) algorithm.

Put slightly more formally, recall that the M-step of the standard EM algorithm performs the maximization

$$\theta := \arg\max_\theta \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$$

The GEM algorithm, in constrast, performs the following update in the M-step:

$$\theta := \theta + \alpha \nabla_\theta \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}$$

where α is a learning rate which we assume is choosen small enough such that we do not decrease the objective function when taking this gradient step.

(a) Prove that the GEM algorithm described above converges. To do this, you should show that the the likelihood is monotonically improving, as it does for the EM algorithm — i.e., show that $\ell(\theta^{(t+1)}) \geq \ell(\theta^{(t)})$.

Answer: We use the same logic as for the standard EM algorithm. Specifically, just as for EM, we have for the GEM algorithm that

$$\begin{aligned} \ell(\theta^{(t+1)}) &\geq \sum_i \sum_{z^{(i)}} Q_i^{(t)}(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta^{(t+1)})}{Q_i^{(t)}(z^{(i)})} \\ &\geq \sum_i \sum_{z^{(i)}} Q_i^{(t)}(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta^{(t)})}{Q_i^{(t)}(z^{(i)})} \\ &= \ell(\theta^{(t)}) \end{aligned}$$

where as in EM the first line holds due to Jensen's equality, and the last line holds because we choose the Q distribution to make this hold with equality. The only difference between EM and GEM is the logic as to why the second line holds: for EM it held because $\theta^{(t+1)}$ was chosen to maximize this quantity, but for GEM it holds by our assumption that we take a gradient step small enough so as not to decrease the objective function.

(b) Instead of using the EM algorithm at all, suppose we just want to apply gradient ascent to maximize the log-likelihood directly. In other words, we are trying to maximize the (non-convex) function

$$\ell(\theta) = \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta)$$

so we could simply use the update

$$\theta := \theta + \alpha \nabla_\theta \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta).$$

Show that this procedure in fact gives the same update as the GEM algorithm described above.

Answer: Differentiating the log likelihood directly we get

$$\begin{aligned} \frac{\partial}{\partial \theta_j} \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta) &= \sum_i \frac{1}{\sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta)} \sum_{z^{(i)}} \frac{\partial}{\partial \theta_j} p(x^{(i)}, z^{(i)}; \theta) \\ &= \sum_i \sum_{z^{(i)}} \frac{1}{p(x^{(i)}; \theta)} \cdot \frac{\partial}{\partial \theta_j} p(x^{(i)}, z^{(i)}; \theta). \end{aligned}$$

For the GEM algorithm,

$$\frac{\partial}{\partial \theta_j} \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})} \quad = \quad \sum_i \sum_{z^{(i)}} \frac{Q_i(z^{(i)})}{p(x^{(i)}, z^{(i)}; \theta)} \cdot \frac{\partial}{\partial \theta_j} p(x^{(i)}, z^{(i)}; \theta).$$

But the E-step of the GEM algorithm chooses

$$Q_i(z^{(i)}) = p(z^{(i)} | x^{(i)}; \theta) = \frac{p(x^{(i)}, z^{(i)}; \theta)}{p(x^{(i)}; \theta)},$$

so

$$\sum_i \sum_{z^{(i)}} \frac{Q_i(z^{(i)})}{p(x^{(i)}, z^{(i)}; \theta)} \cdot \frac{\partial}{\partial \theta_j} p(x^{(i)}, z^{(i)}; \theta) = \sum_i \sum_{z^{(i)}} \frac{1}{p(x^{(i)}; \theta)} \cdot \frac{\partial}{\partial \theta_j} p(x^{(i)}, z^{(i)}; \theta)$$

which is the same as the derivative of the log likelihood.

CS 229, Public Course Problem Set #4: Unsupervised Learning and Reinforcement Learning

1. **EM for supervised learning**

   In class we applied EM to the unsupervised learning setting. In particular, we represented $p(x)$ by marginalizing over a latent random variable

$$p(x) = \sum_z p(x,z) = \sum_z p(x|z)p(z).$$

   However, EM can also be applied to the supervised learning setting, and in this problem we discuss a "mixture of linear regressors" model; this is an instance of what is often call the Hierarchical Mixture of Experts model. We want to represent $p(y|x)$, $x \in \mathbb{R}^n$ and $y \in \mathbb{R}$, and we do so by again introducing a discrete latent random variable

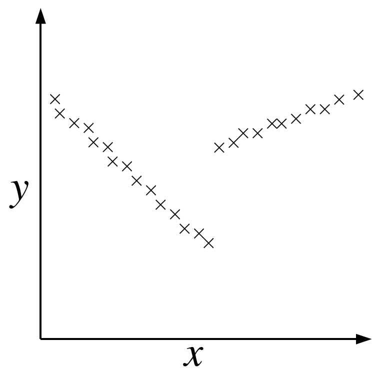
$$p(y|x) = \sum_z p(y,z|x) = \sum_z p(y|x,z)p(z|x).$$

   For simplicity we'll assume that z is binary valued, that $p(y|x,z)$ is a Gaussian density, and that $p(z|x)$ is given by a logistic regression model. More formally

$$\begin{aligned} p(z|x;\phi) &= g(\phi^T x)^z (1 - g(\phi^T x))^{1-z} \\ p(y|x,z=i;\theta_i) &= \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(y - \theta_i^T x)^2}{2\sigma^2} \right) \qquad i = 1,2 \end{aligned}$$

   where σ is a known parameter and $\phi, \theta_0, \theta_1 \in \mathbb{R}^n$ are parameters of the model (here we use the subscript on θ to denote two different parameter vectors, not to index a particular entry in these vectors).

   Intuitively, the process behind model can be thought of as follows. Given a data point x, we first determine whether the data point belongs to one of two hidden classes $z = 0$ or $z = 1$, using a logistic regression model. We then determine y as a linear function of x (different linear functions for different values of z) plus Gaussian noise, as in the standard linear regression model. For example, the following data set could be well-represented by the model, but not by standard linear regression.



(a) Suppose x, y, and z are all observed, so that we obtain a training set $\{(x^{(1)}, y^{(1)}, z^{(1)}), \ldots, (x^{(m)}, y^{(m)}, z^{(m)})\}$. Write the log-likelihood of the parameters, and derive the maximum likelihood estimates for ϕ, θ_0, and θ_1. Note that because $p(z|x)$ is a logistic regression model, there will not exist a closed form estimate of ϕ. In this case, derive the gradient and the Hessian of the likelihood with respect to ϕ; in practice, these quantities can be used to numerically compute the ML esimtate.

(b) Now suppose z is a latent (unobserved) random variable. Write the log-likelihood of the parameters, and derive an EM algorithm to maximize the log-likelihood. Clearly specify the E-step and M-step (again, the M-step will require a numerical solution, so find the appropriate gradients and Hessians).

2. **Factor Analysis and PCA**

In this problem we look at the relationship between two unsupervised learning algorithms we discussed in class: Factor Analysis and Principle Component Analysis.

Consider the following joint distribution over (x, z) where $z \in \mathbb{R}^k$ is a latent random variable

$$\begin{aligned} z &\sim \mathcal{N}(0, I) \\ x|z &\sim \mathcal{N}(Uz, \sigma^2 I). \end{aligned}$$

where $U \in \mathbb{R}^{n \times k}$ is a model parameters and σ^2 is assumed to be a known constant. This model is often called Probabilistic PCA. Note that this is nearly identical to the factor analysis model except we assume that the variance of $x|z$ is a known scaled identity matrix rather than the diagonal parameter matrix, Φ, and we do not add an additional μ term to the mean (though this last difference is just for simplicity of presentation). However, as we will see, it turns out that as $\sigma^2 \to 0$, this model is equivalent to PCA.

For simplicity, you can assume for the remainder of the problem that $k = 1$, i.e., that U is a column vector in $\mathbb{R}^n$.

(a) Use the rules for manipulating Gaussian distributions to determine the joint distribution over (x, z) and the conditional distribution of $z|x$. [Hint: for later parts of this problem, it will help significantly if you simplify your soluting for the conditional distribution using the identity we first mentioned in problem set #1: $(\lambda I + BA)^{-1}B = B(\lambda I + AB)^{-1}$.]

(b) Using these distributions, derive an EM algorithm for the model. Clearly state the E-step and the M-step of the algorithm.

(c) As $\sigma^2 \to 0$, show that if the EM algorithm convergences to a parameter vector $U^\star$ (and such convergence is guarenteed by the argument presented in class), then $U^\star$ must be an eigenvector of the sample covariance matrix $\Sigma = \frac{1}{m}\sum_{i=1}^m x^{(i)} {x^{(i)}}^T$ — i.e., $U^\star$ must satisfy

$$\lambda U^\star = \Sigma U^\star.$$

[Hint: When $\sigma^2 \to 0$, $\Sigma_{z|x} \to 0$, so the E step only needs to compute the means $\mu_{z|x}$ and not the variances. Let $w \in \mathbb{R}^m$ be a vector containing all these means, $w_i = \mu_{z^{(i)}|x^{(i)}}$, and show that the E step and M step can be expressed as

$$w = \frac{XU}{U^T U}, \quad U = \frac{X^T w}{w^T w}$$

respectively. Finally, show that if U doesn't change after this update, it must satisfy the eigenvector equation shown above.]

3. **PCA and ICA for Natural Images**

   In this problem we'll apply Principal Component Analysis and Independent Component Analysis to images patches collected from "natural" image scenes (pictures of leaves, grass, etc). This is one of the classical applications of the ICA algorithm, and sparked a great deal of interest in the algorithm; it was observed that the bases recovered by ICA closely resemble image filters present in the first layer of the visual cortex.

   The `q3/` directory contains the data and several useful pieces of code for this problem. The raw images are stored in the *images/* subdirectory, though you will not need to work with these directly, since we provide code for loading and normalizing the images.

   Calling the function `[X_ica, X_pca] = load_images;` will load the images, break them into 16x16 images patches, and place all these patches into the columns of the matrices `X_ica` and `X_pca`. We create two different data sets for PCA and ICA because the algorithms require slightly different methods of preprocessing the data.[1]

   For this problem you'll implement the `ica.m` and `pca.m` functions, using the PCA and ICA algorithms described in the class notes. While the PCA implementation should be straightforward, getting a good implementation of ICA can be a bit trickier. Here is some general advice to getting a good implementation on this data set:

   - Picking a good learning rate is important. In our experiments we used $\alpha = 0.0005$ on this data set.
   - Batch gradient descent doesn't work well for ICA (this has to do with the fact that ICA objective function is not concave), but the pure stochastic gradient described in the notes can be slow (There are about 20,000 16x16 images patches in the data set, so one pass over the data using the stochastic gradient rule described in the notes requires inverting the 256x256 W matrix 20,000 times). Instead, a good compromise is to use a hybrid stochastic/batch gradient descent where we calculate the gradient with respect to several examples at a time (100 worked well for us), and use this to update W. Our implementation makes 10 total passes over the entire data set.
   - It is a good idea to randomize the order of the examples presented to stochastic gradient descent before each pass over the data.
   - Vectorize your Matlab code as much as possible. For general examples of how to do this, look at the Matlab review session.

   For reference, computing the ICA W matrix for the entire set of image patches takes about 5 minutes on a 1.6 Ghz laptop using our implementation.

   After you've learned the U matrix for PCA (the columns of U should contain the principal components of the data) and the W matrix of ICA, you can plot the basis functions using the `plot_ica_bases(W);` and `plot_pca_bases(U);` functions we have provide. Comment briefly on the difference between the two sets of basis functions.

[1] Recall that the first step of performing PCA is to subtract the mean and normalize the variance of the features. For the image data we're using, the preprocessing step for the ICA algorithm is slightly different, though the precise mechanism and justification is not imporant for the sake of this problem. Those who are curious about the details should read Bell and Sejnowki's paper "The 'Independent Components' of Natural Scenes are Edge Filters," which provided the basis for the implementation we use in this problem.

4. **Convergence of Policy Iteration**

   In this problem we show that the Policy Iteration algorithm, described in the lecture notes, is guarenteed to find the optimal policy for an MDP. First, define B^π to be the Bellman operator for policy π, defined as follows: if $V' = B(V)$, then

$$V'(s) = R(s) + \gamma \sum_{s' \in \mathcal{S}} P_{s\pi(s)}(s')V(s').$$

   (a) Prove that if $V_1(s) \leq V_2(s)$ for all $s \in \mathbb{S}$, then $B(V_1)(s) \leq B(V_2)(s)$ for all $s \in \mathbb{S}$.

   (b) Prove that for any V,

$$\|B^\pi(V) - V^\pi\|_\infty \leq \gamma \|V - V^\pi\|_\infty$$

   where $\|V\|_\infty = \max_{s \in \mathcal{S}} |V(s)|$. Intuitively, this means that applying the Bellman operator B^π to any value function V, brings that value function "closer" to the value function for π, V^π. This also means that applying B^π repeatedly (an infinite number of times)

$$B^\pi(B^\pi(\dots B^\pi(V)\dots))$$

   will result in the value function V^π (a little bit more is needed to make this completely formal, but we won't worry about that here).

   [Hint: Use the fact that for any $\alpha, x \in \mathbb{R}^n$, if $\sum_i \alpha_i = 1$ and $\alpha_i \geq 0$, then $\sum_i \alpha_i x_i \leq \max_i x_i$.]

   (c) Now suppose that we have some policy π, and use Policy Iteration to choose a new policy π' according to

$$\pi'(s) = \arg\max_{a \in \mathcal{A}} \sum_{s' \in \mathcal{S}} P_{sa}(s')V^\pi(s').$$

   Show that this policy will never perform worse that the previous one — i.e., show that for all $s \in \mathcal{S}$, $V^\pi(s) \leq V^{\pi'}(s)$.

   [Hint: First show that $V^\pi(s) \leq B^{\pi'}(V^\pi)(s)$, then use the proceeding excercises to show that $B^{\pi'}(V^\pi)(s) \leq V^{\pi'}(s)$.]

   (d) Use the proceeding exercises to show that policy iteration will eventually converge (i.e., produce a policy $\pi' = \pi$). Furthermore, show that it must converge to the optimal policy $\pi^\star$. For the later part, you may use the property that if some value function satisfies

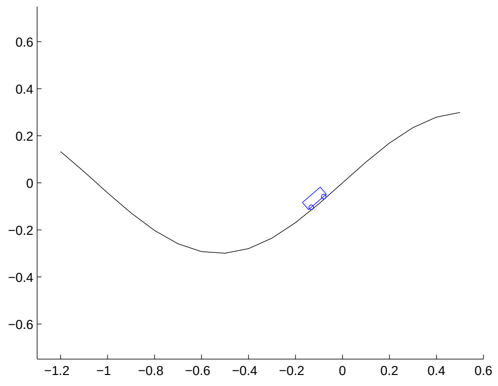
$$V(s) = R(s) + \gamma \max_{a \in \mathcal{A}} \sum s' \in \mathcal{S} P_{sa}(s')V(s')$$

   then $V = V^\star$.

5. **Reinforcement Learning: The Mountain Car**

   In this problem you will implement the Q-Learning reinforcement learning algorithm described in class on a standard control domain known as the Mountain Car.[2] The Mountain Car domain simulates a car trying to drive up a hill, as shown in the figure below.

[2]The dynamics of this domain were taken from Sutton and Barto, 1998.



All states except those at the top of the hill have a constant reward $R(s) = -1$, while the goal state at the hilltop has reward $R(s) = 0$; thus an optimal agent will try to get to the top of the hill as fast as possible (when the car reaches the top of the hill, the episode is over, and the car is reset to its initial position). However, when starting at the bottom of the hill, the car does not have enough power to reach the top by driving forward, so it must first accerlaterate accelerate backwards, building up enough momentum to reach the top of the hill. This strategy of moving away from the goal in order to reach the goal makes the problem difficult for many classical control algorithms.

As discussed in class, Q-learning maintains a table of Q-values, $Q(s, a)$, for each state and action. These Q-values are useful because, in order to select an action in state s, we only need to check to see which Q-value is greatest. That is, in state s we take the action

$$\arg\max_{a \in \mathcal{A}} Q(s, a).$$

The Q-learning algorithm adjusts its estimates of the Q-values as follows. If an agent is in state s, takes action a, then ends up in state s', Q-learning will update $Q(s, a)$ by

$$Q(s, a) = (1 - \alpha)Q(s, a) + \gamma(R(s') + \gamma \max_{a' \in \mathcal{A}} Q(s', a').$$

At each time, your implementation of Q-learning can execute the greedy policy $\pi(s) = \arg\max_{a \in \mathcal{A}} Q(s, a)$

Implement the `[q, steps_per_episode] = qlearning(episodes)` function in the `q5/` directory. As input, the function takes the total number of episodes (each episode starts with the car at the bottom of the hill, and lasts until the car reaches the top), and outputs a matrix of the Q-values and a vector indicating how many steps it took before the car was able to reach the top of the hill. You should use the `[x, s, absorb] = mountain_car(x, actions(a))` function to simulate one control cycle for the task — the `x` variable describes the true (continuous) state of the system, whereas the `s` variable describes the discrete index of the state, which you'll use to build the Q values.

Plot a graph showing the average number of steps before the car reaches the top of the hill versus the episode number (there is quite a bit of variation in this quantity, so you will probably want to average these over a large number of episodes, as this will give you a better idea of how the number of steps before reaching the hilltop is decreasing). You can also visualize your resulting controller by calling the `draw_mountain_car(q)` function.

CS 229, Public Course
Problem Set #4 Solutions: Unsupervised Learning and Reinforcement Learning

1. **EM for supervised learning**

   In class we applied EM to the unsupervised learning setting. In particular, we represented $p(x)$ by marginalizing over a latent random variable

$$p(x) = \sum_z p(x, z) = \sum_z p(x|z)p(z).$$

   However, EM can also be applied to the supervised learning setting, and in this problem we discuss a "mixture of linear regressors" model; this is an instance of what is often call the Hierarchical Mixture of Experts model. We want to represent $p(y|x)$, $x \in \mathbb{R}^n$ and $y \in \mathbb{R}$, and we do so by again introducing a discrete latent random variable

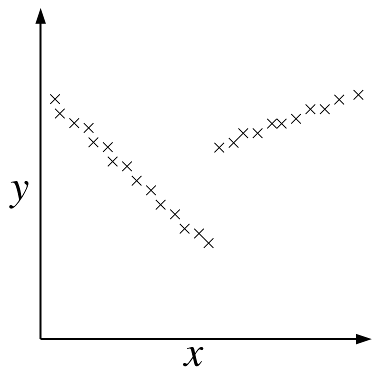
$$p(y|x) = \sum_z p(y, z|x) = \sum_z p(y|x, z)p(z|x).$$

   For simplicity we'll assume that z is binary valued, that $p(y|x, z)$ is a Gaussian density, and that $p(z|x)$ is given by a logistic regression model. More formally

$$\begin{aligned} p(z|x; \phi) &= g(\phi^T x)^z (1 - g(\phi^T x))^{1-z} \\ p(y|x, z = i; \theta_i) &= \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(y - \theta_i^T x)^2}{2\sigma^2}\right) \quad i = 1, 2 \end{aligned}$$

   where σ is a known parameter and $\phi, \theta_0, \theta_1 \in \mathbb{R}^n$ are parameters of the model (here we use the subscript on θ to denote two different parameter vectors, not to index a particular entry in these vectors).

   Intuitively, the process behind model can be thought of as follows. Given a data point x, we first determine whether the data point belongs to one of two hidden classes $z = 0$ or $z = 1$, using a logistic regression model. We then determine y as a linear function of x (different linear functions for different values of z) plus Gaussian noise, as in the standard linear regression model. For example, the following data set could be well-represented by the model, but not by standard linear regression.



(a) Suppose x, y, and z are all observed, so that we obtain a training set $\{(x^{(1)}, y^{(1)}, z^{(1)}), \ldots, (x^{(m)}, y^{(m)}, z^{(m)})\}$. Write the log-likelihood of the parameters, and derive the maximum likelihood estimates for ϕ, θ_0, and θ_1. Note that because $p(z|x)$ is a logistic regression model, there will not exist a closed form estimate of ϕ. In this case, derive the gradient and the Hessian of the likelihood with respect to ϕ; in practice, these quantities can be used to numerically compute the ML esimtate.

Answer: The log-likelihood is given by

$$\begin{aligned}\ell(\phi, \theta_0, \theta 1) &= \log \prod_{i=1}^{m} p(y^{(i)}|x^{(i)}, z^{(i)}; \theta_0, \theta_1) p(z^{(i)}|x^{(i)}; \phi) \\ &= \sum_{i:z^{(i)}=0} \log \left((1 - g(\phi^T x)) \frac{1}{\sqrt{2\pi}\sigma} \exp \left(\frac{-(y^{(i)} - \theta_0^T x^{(i)})^2}{2\sigma^2} \right) \right) \\ &\quad + \sum_{i:z^{(i)}=1} \log \left((g(\phi^T x) \frac{1}{\sqrt{2\pi}\sigma} \exp \left(\frac{-(y^{(i)} - \theta_1^T x^{(i)})^2}{2\sigma^2} \right) \right)\end{aligned}$$

Differentiating with respect to θ_1 and setting it to 0,

$$\begin{aligned}0 &\overset{\text{set}}{=} \nabla_{\theta_0} \ell(\phi, \theta_0, \theta_1) \\ &= \nabla_\theta \sum_{i:z^{(i)}=0} -(y^{(i)} - \theta_0^T x^{(i)})^2\end{aligned}$$

But this is just a least-squares problem on a subset of the data. In particular, if we let X_0 and $\vec{y}_0$ be the design matrices formed by considering only those examples with $z^{(i)} = 0$, then using the same logic as for the derivation of the least squares solution we get the maximum likelihood estimate of θ_0,

$$\theta_0 = (X_0^T X_0)^{-1} X_0^T \vec{y}_0.$$

The derivation for θ_1 proceeds in the identical manner.

Differentiating with respect to ϕ, and ignoring terms that do not depend on ϕ

$$\begin{aligned}\nabla_\phi \ell(\phi, \theta_0, \theta_1) &= \nabla_\phi \sum i : z^{(i)} = 0 \log(1 - g(\phi^T x)) + \sum i : z^{(i)} = 1 \log g(\phi^T x) \\ &= \nabla_\phi \sum_{i=1}^{m} (1 - z^{(i)}) \log(1 - g(\phi^T x)) + z^{(i)} \log g(\phi^T x)\end{aligned}$$

This is just the standard logistic regression objective function, for which we already know the gradient and Hessian

$$\nabla_\phi \ell(\phi, \theta_0, \theta_1) = X^T(\vec{z} - \vec{h}), \quad \vec{h}_i = g(\phi^T x^{(i)}),$$

$$H = X^T D X, \quad D_{ii} = g(\phi^T x^{(i)})(1 - g(\phi^T x^{(i)})).$$

(b) Now suppose z is a latent (unobserved) random variable. Write the log-likelihood of the parameters, and derive an EM algorithm to maximize the log-likelihood. Clearly specify the E-step and M-step (again, the M-step will require a numerical solution, so find the appropriate gradients and Hessians).

Answer: The log likelihood is now:

$$\begin{aligned}
\ell(\phi, \theta_0, \theta_1) &= \log \prod_{i=1}^{m} \sum_{z^{(i)}} p(y^{(i)}|x^{(i)}, z^{(i)}; \theta_1, \theta_2) p(z^{(i)}|x^{(i)}; \phi) \\
&= \sum_{i=1}^{m} \log \left((1 - g(\phi^T x^{(i)}))^{1-z^{(i)}} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(y^{(i)} - \theta_0^T x^{(i)})^2}{2\sigma^2} \right) \right. \\
&\qquad \left. + \, g(\phi^T x^{(i)})^{z^{(i)}} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{-(y^{(i)} - \theta_1^T x^{(i)})^2}{2\sigma^2} \right) \right)
\end{aligned}$$

In the E-step of the EM algorithm we compute

$$Q_i(z^{(i)}) = p(z^{(i)}|x^{(i)}, y^{(i)}; \phi, \theta_0, \theta_1) = \frac{p(y^{(i)}|x^{(i)}, z^{(i)}; \theta_0, \theta_1) p(z^{(i)}|x^{(i)}; \phi)}{\sum_z p(y^{(i)}|x^{(i)}, z; \theta_0, \theta_1) p(z|x^{(i)}; \phi)}$$

Every propability in this term can be computed using the probability densities defined in the problem, so the E-step is tractable.

For the M-step, we first define $w_j^{(i)} = p(z^{(i)} = j|x^{(i)}, y^{(i)}; \phi, \theta_0, \theta_1)$ for $j = 0, 1$ as computed in the E-step (of course we only need to compute one of these terms in the real E-step, since $w_0^{(i)} = 1 - w_1^{(i)}$, but we define both to simplify the expressions). Differentiating our lower bound on the likelihood with respect to θ_0, removing terms that don't depend on θ_0, and setting the expression equal to zero, we get

$$\begin{aligned}
0 &\overset{\text{set}}{=} \nabla_{\theta_0} \sum_{i=1}^{m} \sum_{j=0,1} w_j^{(i)} \log \frac{p(y^{(i)}|x^{(i)}, z^{(i)} = j; \theta_j) p(z^{(i)} = j|x^{(i)}; \phi)}{w_j^{(i)}} \\
&= \nabla_{\theta_0} \sum_{i=1}^{m} w_0^{(i)} \log p(y^{(i)}|x^{(i)}, z^{(i)} = j; \theta_j) \\
&= \nabla_{\theta_0} \sum_{i=1}^{m} -w_0^{(i)} (y^{(i)} - \theta_0^T x^{(i)})^2
\end{aligned}$$

This is just a weighted least-squares problem, which has solution

$$\theta_0 = (X_0^T W X_0)^{-1} X_0^T W \vec{y}_0, \qquad W = \operatorname{diag}(w_0^{(1)}, \ldots, w_0^{(m)}.$$

The derivation for θ_1 proceeds similarly.

Finally, as before, we can't compute the M-step update for ϕ in closed form, so we instead find the gradient and Hessian. However, to do this we note that

$$\nabla_\phi \sum_{i=1}^{m} \sum_{j=0,1} w_j^{(i)} \log \frac{p(y^{(i)}|x^{(i)}, z^{(i)} = j; \theta_j) p(z^{(i)} = j|x^{(i)}; \phi)}{w_j^{(i)}} =$$

$$\nabla_\phi \sum_{i=1}^{m} \sum_{j=0,1} w_j^{(i)} \log p(z^{(i)} = j|x^{(i)}; \phi) = \sum_{i=1}^{m} \left(w_0^{(i)} \log g(\phi^T x) + (1 - w_0^{(i)}) \log(1 - g(\phi^T x^{(i)})) \right)$$

This term is the same as the objective for logistic regression task, but with the $w^{(i)}$ quantity replacing $y^{(i)}$. Therefore, the gradient and Hessian are given by

$$\nabla_\phi \sum_{i=1}^{m} \sum_{j=0,1} w_j^{(i)} \log p(z^{(i)} = j | x^{(i)}; \phi) = X^T(\vec{w} - \vec{h}), \quad \vec{h}_i = g(\phi^T x^{(i)}),$$
$$H = X^T D X, \quad D_{ii} = g(\phi^T x^{(i)})(1 - g(\phi^T x^{(i)})).$$

2. **Factor Analysis and PCA**

In this problem we look at the relationship between two unsupervised learning algorithms we discussed in class: Factor Analysis and Principle Component Analysis.

Consider the following joint distribution over (x, z) where $z \in \mathbb{R}^k$ is a latent random variable

$$\begin{aligned} z &\sim \mathcal{N}(0, I) \\ x|z &\sim \mathcal{N}(Uz, \sigma^2 I). \end{aligned}$$

where $U \in \mathbb{R}^{n \times k}$ is a model parameters and σ^2 is assumed to be a known constant. This model is often called Probabilistic PCA. Note that this is nearly identical to the factor analysis model except we assume that the variance of $x|z$ is a known scaled identity matrix rather than the diagonal parameter matrix, Φ, and we do not add an additional μ term to the mean (though this last difference is just for simplicity of presentation). However, as we will see, it turns out that as $\sigma^2 \to 0$, this model is equivalent to PCA.

For simplicity, you can assume for the remainder of the problem that $k = 1$, i.e., that U is a column vector in $\mathbb{R}^n$.

(a) Use the rules for manipulating Gaussian distributions to determine the joint distribution over (x, z) and the conditional distribution of $z|x$. [Hint: for later parts of this problem, it will help significantly if you simplify your soluting for the conditional distribution using the identity we first mentioned in problem set #1: $(\lambda I + BA)^{-1}B = B(\lambda I + AB)^{-1}$.]

Answer: To compute the joint distribution, we compute the means and covariances of x and z. First, $E[z] = 0$ and

$$E[x] = E[Uz + \epsilon] = UE[z] + E[\epsilon] = 0, \quad \text{(where } \epsilon \sim \mathcal{N}(0, \sigma^2 I)\text{)}.$$

Since both x and z have zero mean

$$\begin{aligned} \Sigma_{zz} &= E[zz^T] = I \quad (= 1\text{, since } z \text{ is a scalar when } k = 1) \\ \Sigma_{zx} &= E[(Uz + \epsilon)z^T] = UE[zz^T] + E[\epsilon z^T] = U \\ \Sigma_{xx} &= E[(Uz + \epsilon)(Uz + \epsilon)^T] = E[Uzz^TU^T + \epsilon z^T U^T + Uz\epsilon^T + \epsilon\epsilon^T] \\ &= UE[zz^T]U^T + E[\epsilon\epsilon^T] = UU^T + \sigma^2 I \end{aligned}$$

Therefore,

$$\begin{bmatrix} z \\ x \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & U^T \\ U & UU^T + \sigma^2 I \end{bmatrix} \right).$$

Using the rules for conditional Gaussian distributions, $z|x$ is also Gaussian with mean and covariance

$$\begin{aligned} \mu_{z|x} &= U^T(UU^T + \sigma^2 I)^{-1} x = \frac{U^T x}{U^T U + \sigma^2} \\ \Sigma_{z|x} &= 1 - U^T(UU^T + \sigma^2 I)^{-1} U = 1 - \frac{U^T U}{U^T U + \sigma^2} \end{aligned}$$

where in both cases the last equality comes from the identity in the hint.

(b) Using these distributions, derive an EM algorithm for the model. Clearly state the E-step and the M-step of the algorithm.

Answer: Even though $z^{(i)}$ is a scalar value, in this problem we continue to use the notation $z^{(i)^T}$, etc, to make the similarities to the Factor anlysis case obvious.

For the E-step, we compute the distribution $Q_i(z^{(i)}) = p(z^{(i)}|x^{(i)}; U)$ by computing $\mu_{z^{(i)}|x^{(i)}}$ and $\Sigma_{z^{(i)}|x^{(i)}}$ using the above formulas.

For the M-step, we need to maximize

$$\sum_{i=1}^{m} \int_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, |z^{(i)}; U)p(z^{(i)})}{Q_i(z^{(i)})}$$

$$= \sum_{i=1}^{m} E_{z^{(i)} \sim Q_i} \left[\log p(x^{(i)}|z^{(i)}; U) + \log p(z^{(i)}) - \log Q_i(z^{(i)}) \right].$$

Taking the gradient with respect to U equal to zero, dropping terms that don't depend on U, and omitting the subscript on the expectation, this becomes

$$\begin{aligned}
\nabla_U \sum_{i=1}^{m} E\left[\log p(x^{(i)}|z^{(i)}; U)\right] &= \nabla_U \sum_{i=1}^{m} E\left[-\frac{1}{2\sigma^2}(x^{(i)} - Uz^{(i)})^T(x^{(i)} - Uz^{(i)})\right] \\
&= -\frac{1}{2\sigma^2} \sum_{i=1}^{m} \nabla_U E\left[\mathrm{tr} z^{(i)^T} U^T U z^{(i)} - 2\mathrm{tr} z^{(i)^T} U^T x^{(i)}\right] \\
&= -\frac{1}{2\sigma^2} \sum_{i=1}^{m} E\left[Uz^{(i)} z^{(i)^T} - x^{(i)} z^{(i)^T}\right] \\
&= \frac{1}{2\sigma^2} \sum_{i=1}^{m} \left[-UE[z^{(i)} z^{(i)^T}] + x^{(i)} E[z^{(i)^T}]\right]
\end{aligned}$$

using the same reasoning as in the Factor Analysis class notes. Setting this derivative to zero gives

$$\begin{aligned}
U &= \left(\sum_{i=1}^{m} x^{(i)} E[z^{(i)^T}]\right)\left(\sum_{i=1}^{m} E[z^{(i)} z^{(i)^T}]\right)^{-1} \\
&= \left(\sum_{i=1}^{m} x^{(i)} \mu^T_{z^{(i}|x^{(i)}}\right)\left(\sum_{i=1}^{m} \Sigma_{z^{(i)}|x^{(i)}} + \mu_{z^{(i}|x^{(i)}} \mu^T_{z^{(i}|x^{(i)}}\right)^{-1}
\end{aligned}$$

All these terms were calcuated in the E step, so this is our final M step update.

(c) As $\sigma^2 \to 0$, show that if the EM algorithm convergences to a parameter vector $U^\star$ (and such convergence is guarenteed by the argument presented in class), then $U^\star$ must be an eigenvector of the sample covariance matrix $\Sigma = \frac{1}{m}\sum_{i=1}^{m} x^{(i)} x^{(i)^T}$ — i.e., $U^\star$ must satisfy

$$\lambda U^\star = \Sigma U^\star.$$

[Hint: When $\sigma^2 \to 0$, $\Sigma_{z|x} \to 0$, so the E step only needs to compute the means $\mu_{z|x}$ and not the variances. Let $w \in \mathbb{R}^m$ be a vector containing all these means,

$w_i = \mu_{z^{(i)}|x^{(i)}}$, and show that the E step and M step can be expressed as

$$w = \frac{XU}{U^TU}, \quad U = \frac{X^Tw}{w^Tw}$$

respectively. Finally, show that if U doesn't change after this update, it must satisfy the eigenvector equation shown above.]

Answer: For the E step, when $\sigma^2 \to 0$, $\mu_{z^{(i)}|x^{(i)}} = \frac{U^Tx^{(i)}}{U^TU}$, so using w as defined in the hint we have

$$w = \frac{XU}{U^TU}$$

as desired.

As mentioned in the hint, when $\sigma^2 \to 0$, $\Sigma_{z^{(i)}|x^{(i)}} = 0$, so

$$\begin{aligned} U &= \left(\sum_{i=1}^m x^{(i)}\mu^T_{z^{(i}|x^{(i)}}\right)\left(\sum_{i=1}^m \Sigma_{z^{(i)}|x^{(i)}} + \mu_{z^{(i}|x^{(i)}}\mu^T_{z^{(i}|x^{(i)}}\right)^{-1} \\ &= \left(\sum_{i=1}^m x^{(i)}w_i\right)(\sum_{i=1}^m w_iw_i)^{-1} = \frac{X^Tw}{w^Tw} \end{aligned}$$

For U to remain unchanged after an update requires that

$$U = \frac{X^T\frac{XU}{U^TU}}{\frac{U^TX^T}{U^TU}\frac{XU}{U^TU}} = X^TXU\frac{U^TU}{U^TX^TXU} = X^TXU\frac{1}{\lambda}$$

proving the desired equation.

3. **PCA and ICA for Natural Images**

In this problem we'll apply Principal Component Analysis and Independent Component Analysis to images patches collected from "natural" image scenes (pictures of leaves, grass, etc). This is one of the classical applications of the ICA algorithm, and sparked a great deal of interest in the algorithm; it was observed that the bases recovered by ICA closely resemble image filters present in the first layer of the visual cortex.

The `q3/` directory contains the data and several useful pieces of code for this problem. The raw images are stored in the *images/* subdirectory, though you will not need to work with these directly, since we provide code for loading and normalizing the images.

Calling the function `[X_ica, X_pca] = load_images;` will load the images, break them into 16x16 images patches, and place all these patches into the columns of the matrices `X_ica` and `X_pca`. We create two different data sets for PCA and ICA because the algorithms require slightly different methods of preprocessing the data.[1]

For this problem you'll implement the `ica.m` and `pca.m` functions, using the PCA and ICA algorithms described in the class notes. While the PCA implementation should be straightforward, getting a good implementation of ICA can be a bit trickier. Here is some general advice to getting a good implementation on this data set:

[1]Recall that the first step of performing PCA is to subtract the mean and normalize the variance of the features. For the image data we're using, the preprocessing step for the ICA algorithm is slightly different, though the precise mechanism and justification is not imporant for the sake of this problem. Those who are curious about the details should read Bell and Sejnowki's paper "The 'Independent Components' of Natural Scenes are Edge Filters," which provided the basis for the implementation we use in this problem.

- Picking a good learning rate is important. In our experiments we used $\alpha = 0.0005$ on this data set.
- Batch gradient descent doesn't work well for ICA (this has to do with the fact that ICA objective function is not concave), but the pure stochastic gradient described in the notes can be slow (There are about 20,000 16x16 images patches in the data set, so one pass over the data using the stochastic gradient rule described in the notes requires inverting the 256x256 W matrix 20,000 times). Instead, a good compromise is to use a hybrid stochastic/batch gradient descent where we calculate the gradient with respect to several examples at a time (100 worked well for us), and use this to update W. Our implementation makes 10 total passes over the entire data set.
- It is a good idea to randomize the order of the examples presented to stochastic gradient descent before each pass over the data.
- Vectorize your Matlab code as much as possible. For general examples of how to do this, look at the Matlab review session.

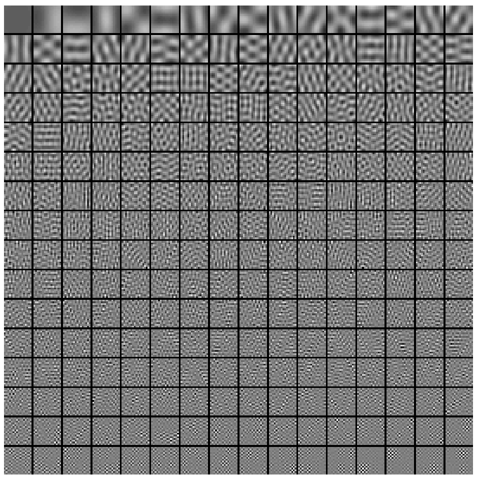
For reference, computing the ICA W matrix for the entire set of image patches takes about 5 minutes on a 1.6 Ghz laptop using our implementation.

After you've learned the U matrix for PCA (the columns of U should contain the principal components of the data) and the W matrix of ICA, you can plot the basis functions using the `plot_ica_bases(W);` and `plot_pca_bases(U);` functions we have provide. Comment briefly on the difference between the two sets of basis functions.

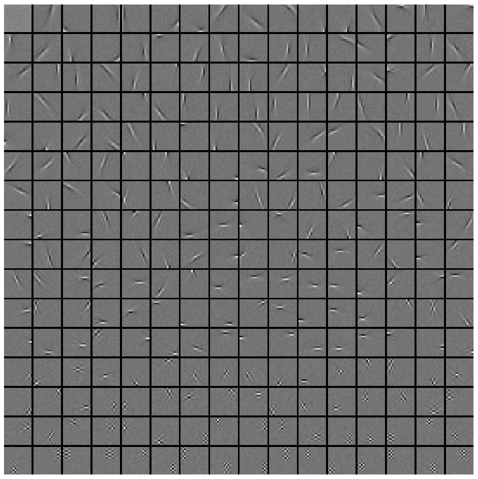
Answer: The following are our implementations of `pca.m` and `ica.m`:

```
function U = pca(X)

[U,S,V] = svd(X*X');

function W = ica(X)

[n,m] = size(X);
chunk = 100;
alpha = 0.0005;
W = eye(n);

for iter=1:10,
  disp([num2str(iter)]);
  X = X(:,randperm(m));
  for i=1:floor(m/chunk),
    Xc = X(:,(i-1)*chunk+1:i*chunk);
    dW = (1 - 2./(1+exp(-W*Xc)))*Xc' + chunk*inv(W');
    W = W + alpha*dW;
  end
end
```

PCA produces the following bases:



while ICA produces the following bases



The PCA bases capture global features of the images, while the ICA bases capture more local features.

4. **Convergence of Policy Iteration**

   In this problem we show that the Policy Iteration algorithm, described in the lecture notes, is guarenteed to find the optimal policy for an MDP. First, define B^π to be the Bellman operator for policy π, defined as follows: if $V' = B(V)$, then

$$V'(s) = R(s) + \gamma \sum_{s' \in \mathcal{S}} P_{s\pi(s)}(s')V(s').$$

(a) Prove that if $V_1(s) \leq V_2(s)$ for all $s \in \mathbb{S}$, then $B(V_1)(s) \leq B(V_2)(s)$ for all $s \in \mathbb{S}$.
Answer:

$$\begin{aligned} B(V_1)(s) &= R(s) + \gamma \sum_{s' \in \mathcal{S}} P_{s\pi(s)}(s')V_1(s') \\ &\leq R(s) + \gamma \sum_{s' \in \mathcal{S}} P_{s\pi(s)}(s')V_2(s') = B(V_2)(s) \end{aligned}$$

where the inequality holds because $P_{s\pi(s)}(s') \geq 0$.

(b) Prove that for any V,

$$\|B^\pi(V) - V^\pi\|_\infty \leq \gamma \|V - V^\pi\|_\infty$$

where $\|V\|_\infty = \max_{s\in\mathcal{S}} |V(s)|$. Intuitively, this means that applying the Bellman operator B^π to any value function V, brings that value function "closer" to the value function for π, V^π. This also means that applying B^π repeatedly (an infinite number of times)

$$B^\pi(B^\pi(\ldots B^\pi(V)\ldots))$$

will result in the value function V^π (a little bit more is needed to make this completely formal, but we won't worry about that here).
[Hint: Use the fact that for any $\alpha, x \in \mathbb{R}^n$, if $\sum_i \alpha_i = 1$ and $\alpha_i \geq 0$, then $\sum_i \alpha_i x_i \leq \max_i x_i$.] **Answer:**

$$\begin{aligned} \|B^\pi(V) - V^\pi\|_\infty &= \max_{s'\in\mathcal{S}} \left| R(s) + \gamma \sum_{s'\in\mathcal{S}} P_{s\pi(s)}(s')V(s') - R(s) - \gamma \sum_{s'\in\mathcal{S}} P_{s\pi(s)}(s')V^\pi(s') \right| \\ &= \gamma \max_{s'\in\int} \left| \sum_{s'\in\mathcal{S}} P_{s\pi(s)}(s')\left(V(s') - V^\pi(s')\right) \right| \\ &\leq \gamma \|V - V^\pi\|_\infty \end{aligned}$$

where the inequality follows from the hint above.

(c) Now suppose that we have some policy π, and use Policy Iteration to choose a new policy π' according to

$$\pi'(s) = \arg\max_{a\in\mathcal{A}} \sum_{s'\in\mathcal{S}} P_{sa}(s')V^\pi(s').$$

Show that this policy will never perform worse that the previous one — i.e., show that for all $s \in \mathcal{S}$, $V^\pi(s) \leq V^{\pi'}(s)$.
[Hint: First show that $V^\pi(s) \leq B^{\pi'}(V^\pi)(s)$, then use the proceeding excercises to show that $B^{\pi'}(V^\pi)(s) \leq V^{\pi'}(s)$.]
Answer:

$$\begin{aligned} V^\pi(s) &= R(s) + \gamma \sum_{s'\in\mathcal{S}} P_{s\pi(s)}(s')V^\pi(s') \\ &\leq R(s) + \gamma \max_{a\in\mathcal{A}} \sum_{s'\in\mathcal{S}} P_{sa}(s')V^\pi(s') \\ &= R(s) + \gamma \sum_{s'\in\mathcal{S}} P_{s\pi'(s)}(s')V^\pi(s') = B^{\pi'}(V^\pi)(s) \end{aligned}$$

Applying part (a),

$$V^{\pi}(s) \le B^{\pi'}(V^{\pi})(s) \Rightarrow B^{\pi'}(V^{\pi})(s) \le B^{\pi'}(B^{\pi'}(V^{\pi}))(s)$$

Continually applying this property, and applying part (b), we obtain

$$V^{\pi}(s) \le B^{\pi'}(V^{\pi})(s) \le B^{\pi'}(B^{\pi'}(V^{\pi}))(s) \le \ldots \le B^{\pi'}(B^{\pi'}(\ldots B^{\pi'}(V^{\pi})\ldots))(s) = V^{\pi'}(s).$$

(d) Use the proceeding exercises to show that policy iteration will eventually converge (i.e., produce a policy $\pi' = \pi$). Furthermore, show that it must converge to the optimal policy $\pi^{\star}$. For the later part, you may use the property that if some value function satisfies

$$V(s) = R(s) + \gamma \max_{a \in \mathcal{A}} \sum s' \in \mathcal{S} P_{sa}(s')V(s')$$

then $V = V^{\star}$.

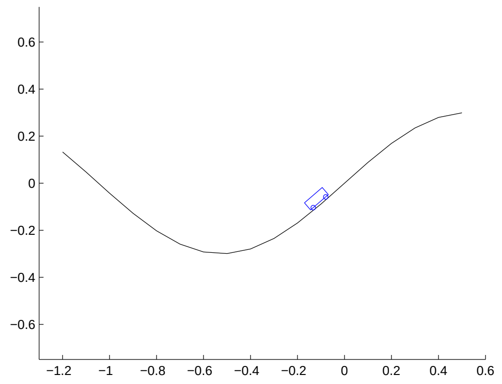
Answer: We know that policy iteration must converge because there are only a finite number of possible policies (if there are $|S|$ states, each with $|A|$ actions, then that leads to a $|S|^{|A|}$ total possible policies). Since the policies are monotonically improving, as we showed in part (c), at some point we must stop generating new policies, so the algorithm must produce $\pi' = \pi$. Using the assumptions stated in the question, it is easy to show convergence to the optimal policy. If $\pi' = \pi$, then using the same logic as in part (c)

$$V^{\pi}(s) = V^{\pi'}(s) = R(s) + \gamma \max_{a \in \mathcal{A}} \sum_{s' \in \int} P_{sa}(s')V^{\pi}(s),$$

So $V = V^{\star}$, and therefore $\pi = \pi^{\star}$.

5. **Reinforcement Learning: The Mountain Car**

In this problem you will implement the Q-Learning reinforcement learning algorithm described in class on a standard control domain known as the Mountain Car.[2] The Mountain Car domain simulates a car trying to drive up a hill, as shown in the figure below.



[2]The dynamics of this domain were taken from Sutton and Barto, 1998.

All states except those at the top of the hill have a constant reward $R(s) = -1$, while the goal state at the hilltop has reward $R(s) = 0$; thus an optimal agent will try to get to the top of the hill as fast as possible (when the car reaches the top of the hill, the episode is over, and the car is reset to its initial position). However, when starting at the bottom of the hill, the car does not have enough power to reach the top by driving forward, so it must first accerlaterate accelerate backwards, building up enough momentum to reach the top of the hill. This strategy of moving away from the goal in order to reach the goal makes the problem difficult for many classical control algorithms.

As discussed in class, Q-learning maintains a table of Q-values, $Q(s, a)$, for each state and action. These Q-values are useful because, in order to select an action in state s, we only need to check to see which Q-value is greatest. That is, in state s we take the action

$$\arg\max_{a \in \mathcal{A}} Q(s, a).$$

The Q-learning algorithm adjusts its estimates of the Q-values as follows. If an agent is in state s, takes action a, then ends up in state s', Q-learning will update $Q(s, a)$ by

$$Q(s, a) = (1 - \alpha)Q(s, a) + \gamma(R(s') + \gamma \max_{a' \in \mathcal{A}} Q(s', a').$$

At each time, your implementation of Q-learning can execute the greedy policy $\pi(s) = \arg\max_{a \in \mathcal{A}} Q(s, a)$

Implement the `[q, steps_per_episode] = qlearning(episodes)` function in the `q5/` directory. As input, the function takes the total number of episodes (each episode starts with the car at the bottom of the hill, and lasts until the car reaches the top), and outputs a matrix of the Q-values and a vector indicating how many steps it took before the car was able to reach the top of the hill. You should use the `[x, s, absorb] = mountain_car(x, actions(a))` function to simulate one control cycle for the task — the `x` variable describes the true (continuous) state of the system, whereas the `s` variable describes the discrete index of the state, which you'll use to build the Q values.

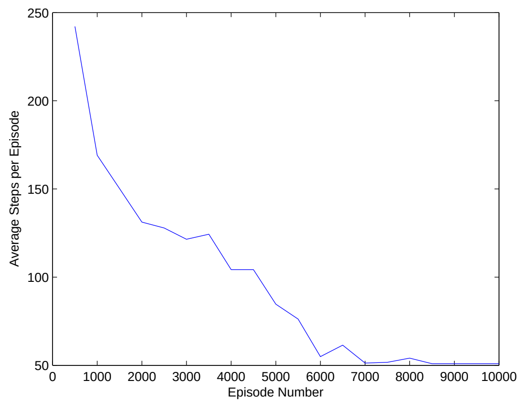
Plot a graph showing the average number of steps before the car reaches the top of the hill versus the episode number (there is quite a bit of variation in this quantity, so you will probably want to average these over a large number of episodes, as this will give you a better idea of how the number of steps before reaching the hilltop is decreasing). You can also visualize your resulting controller by calling the `draw_mountain_car(q)` function.

Answer: The following is our implementation of `qlearning.m`:

```
function [q, steps_per_episode] = qlearning(episodes)

% set up parameters and initialize q values
alpha = 0.05;
gamma = 0.99;
num_states = 100;
num_actions = 2;
actions = [-1, 1];
q = zeros(num_states, num_actions);

for i=1:episodes,
  [x, s, absorb] =  mountain_car([0.0 -pi/6], 0);
  [maxq, a] = max(q(s,:));
  if (q(s,1) == q(s,2)) a = ceil(rand*num_actions); end;
  steps = 0;

  while (~absorb)
    % execute the best action or a random action
    [x, sn, absorb] = mountain_car(x, actions(a));
    reward = -double(absorb == 0);

    % find the best action for the next state and update q value
    [maxq, an] = max(q(sn,:));
    if (q(sn,1) == q(sn,2)) an = ceil(rand*num_actions); end
    q(s,a) = (1 - alpha)*q(s,a) + alpha*(reward + gamma*maxq);
    a = an;
    s = sn;
    steps = steps + 1;
  end
  steps_per_episode(i) = steps;
end
```

Within 10000 episodes, the algorithm converges to a policy that usually gets the car up the hill in around 52-53 steps. The following plot shows the number of steps per episode (averaged over 500 episodes) versus the number of episodes. We generated the plot using the following code:

```
for i=1:10,
  [q, ep_steps] = qlearning(10000);
  all_ep_steps(i,:) = ep_steps;
end
plot(mean(reshape(mean(all_ep_steps), 500, 20)));
```



CS 229, Autumn 2013
Problem Set #1: Supervised Learning

Due in class (9:00am) on Wednesday, October 16.

Notes: (1) These questions require thought, but do not require long answers. Please be as concise as possible. (2) If you have a question about this homework, we encourage you to post your question on our Piazza forum, at `https://piazza.com/stanford/fall2013/cs229`. (3) If you missed the first lecture or are unfamiliar with the collaboration or honor code policy, please read the policy on Handout #1 (available from the course website) before starting work. (4) For problems that require programming, please include in your submission a printout of your code (with comments) and any figures that you are asked to plot. (5) If you are an on-campus (non-SCPD) student, please print, fill out, and include a copy of the cover sheet (enclosed as the final page of this document), and include the cover sheet as the first page of your submission.

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1. **[25 points] Logistic regression**

   (a) [10 points] Consider the log-likelihood function for logistic regression:

   $$\ell(\theta) = \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)}))$$

   Find the Hessian H of this function, and show that for any vector z, it holds true that

   $$z^T H z \leq 0.$$

   [Hint: You might want to start by showing the fact that $\sum_i \sum_j z_i x_i x_j z_j = (x^T z)^2 \geq 0$.]

   Remark: This is one of the standard ways of showing that the matrix H is negative semi-definite, written "$H \leq 0$." This implies that ℓ is concave, and has no local maxima other than the global one.[1] If you have some other way of showing $H \leq 0$, you're also welcome to use your method instead of the one above.

   (b) [10 points] On the Leland system, the files `/afs/ir/class/cs229/ps/ps1/q1x.dat` and `/afs/ir/class/cs229/ps/ps1/q1y.dat` contain the inputs ($x^{(i)} \in \mathbb{R}^2$) and outputs ($y^{(i)} \in \{0, 1\}$) respectively for a binary classification problem, with one training example per row. Implement[2] Newton's method for optimizing $\ell(\theta)$, 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? (Remember to include the intercept term.)

[1] If you haven't seen this result before, please feel encouraged to ask us about it during office hours.
[2] Write your own version, and do not call a built-in library function.

(c) [5 points] 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 0). Also plot on the same figure the decision boundary fit by logistic regression. (I.e., this should be a straight line showing the boundary separating the region where $h(x) > 0.5$ from where $h(x) \leq 0.5$.)

2. **[27 points] 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

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

In class, we worked out what happens for the case where all the weights (the $w^{(i)}$'s) are the same. In this problem, we will generalize some of those ideas to the weighted setting, and also implement the locally weighted linear regression algorithm.

(a) [2 points] Show that $J(\theta)$ can also be written

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

for an appropriate diagonal matrix W, and where X and $\vec{y}$ are as defined in class. State clearly what W is.

(b) [7 points] If all the $w^{(i)}$'s equal 1, then we saw in class that the normal equation is

$$X^T X\theta = X^T \vec{y},$$

and that the value of θ that minimizes $J(\theta)$ is given by $(X^T X)^{-1} X^T \vec{y}$. 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 of X, W and $\vec{y}$.

(c) [6 points] 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.

(d) [12 points] On the Leland computer system, the files `/afs/ir/class/cs229/ps/ps1/q2x.dat` and `/afs/ir/class/cs229/ps/ps1/q2y.dat` contain the inputs ($x^{(i)}$) and outputs ($y^{(i)}$) for a regression problem, with one training example per row.

i. [2 points] Implement (unweighted) linear regression ($y = \theta^T x$) on this dataset (using the normal equations), and plot on the same figure the data and the straight line resulting from your fit. (Remember to include the intercept term.)

ii. [7 points] Implement locally weighted linear regression on this dataset (using the weighted normal equations you derived in part (b)), and plot on the same figure the data and the 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 a bandwidth parameter $\tau = 0.8$. (Again, remember to include the intercept term.)

iii. [3 points] Repeat (ii) four times, with $\tau = 0.1, 0.3, 2$ and 10. Comment **briefly** on what happens to the fit when τ is too small or too large.

3. **[18 points] Poisson regression and the exponential family**

(a) [5 points] 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 $a(\eta)$.

(b) [3 points] 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.)

(c) [10 points] For a training set $\{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$, 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.

(d) **[5 extra credit points]** Consider using GLM with a response variable from any member of the exponential family in which $T(y) = y$, and the canonical response function for the family. Show that stochastic gradient ascent on the log-likelihood $\log p(\vec{y}|X, \theta)$ results in the update rule $\theta_i := \theta_i - \alpha(h(x) - y)x_i$.

4. **[15 points] Gaussian discriminant analysis**

Suppose we are given a dataset $\{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$ consisting of m independent examples, where $x^{(i)} \in \mathbb{R}^n$ are n-dimensional vectors, and $y^{(i)} \in \{0, 1\}$. We will model the joint distribution of (x, y) according to:

$$\begin{aligned}
p(y) &= \phi^y (1-\phi)^{1-y} \\
p(x|y=0) &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1} (x-\mu_0)\right) \\
p(x|y=1) &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1} (x-\mu_1)\right)
\end{aligned}$$

Here, the parameters of our model are ϕ, Σ, μ_0 and μ_1. (Note that while there're two different mean vectors μ_0 and μ_1, there's only one covariance matrix Σ.)

(a) [5 points] Suppose we have already fit ϕ, Σ, μ_0 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

$$p(y=1|x;\phi,\Sigma,\mu_0,\mu_1) = \frac{1}{1+\exp(-\theta^T x)},$$

where θ is some appropriate function of $\phi, \Sigma, \mu_0, \mu_1$. (Note: To get your answer into the form above, for this part of the problem only, you may have to redefine the $x^{(i)}$'s to be $n+1$-dimensional vectors by adding the extra coordinate $x_0^{(i)} = 1$, like we did in class.)

(b) [10 points] 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 $|\Sigma| = \sigma^2$. Given the dataset, we claim that the maximum likelihood estimates of the parameters are given by

$$\begin{aligned}
\phi &= \frac{1}{m}\sum_{i=1}^{m} 1\{y^{(i)}=1\} \\
\mu_0 &= \frac{\sum_{i=1}^{m} 1\{y^{(i)}=0\}x^{(i)}}{\sum_{i=1}^{m} 1\{y^{(i)}=0\}} \\
\mu_1 &= \frac{\sum_{i=1}^{m} 1\{y^{(i)}=1\}x^{(i)}}{\sum_{i=1}^{m} 1\{y^{(i)}=1\}} \\
\Sigma &= \frac{1}{m}\sum_{i=1}^{m}(x^{(i)}-\mu_{y^{(i)}})(x^{(i)}-\mu_{y^{(i)}})^T
\end{aligned}$$

The log-likelihood of the data is

$$\begin{aligned}
\ell(\phi,\mu_0,\mu_1,\Sigma) &= \log\prod_{i=1}^{m} p(x^{(i)},y^{(i)};\phi,\mu_0,\mu_1,\Sigma) \\
&= \log\prod_{i=1}^{m} p(x^{(i)}|y^{(i)};\mu_0,\mu_1,\Sigma)p(y^{(i)};\phi).
\end{aligned}$$

By maximizing ℓ with respect to the four parameters, prove that the maximum likelihood estimates of ϕ, μ_0, μ_1, and Σ are indeed as given in the formulas above. (You may assume that there is at least one positive and one negative example, so that the denominators in the definitions of μ_0 and μ_1 above are non-zero.)

(c) [**5 extra credit points**] Without assuming that $n = 1$, show that the maximum likelihood estimates of ϕ, μ_0, μ_1, and Σ are as given in the formulas in part (b). [Note: If you're fairly sure that you have the answer to this part right, you don't have to do part (b), since that's just a special case.]

5. **[12 points] Linear invariance of optimization 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 $x^{(0)} = \vec{0}$. When the algorithm is run, it will produce a value of $x \in \mathbb{R}^n$ for each iteration: $x^{(1)}, x^{(2)}, \ldots$.

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

(a) [9 points] Show that Newton's method (applied to find the minimum of a function) is invariant to linear reparameterizations. Note that since $z^{(0)} = \vec{0} = A^{-1}x^{(0)}$, it is sufficient to show that if Newton's method applied to $f(x)$ updates $x^{(i)}$ to $x^{(i+1)}$, then Newton's method applied to $g(z)$ will update $z^{(i)} = A^{-1}x^{(i)}$ to $z^{(i+1)} = A^{-1}x^{(i+1)}$.[3]

(b) [3 points] Is gradient descent invariant to linear reparameterizations? Justify your answer.

Reminder: Please include in your submission a printout of your code and figures for the programming questions.

[3]Note that for this problem, you must explicitly prove any matrix calculus identities that you wish to use that are not given in the lecture notes.

CS229: Machine Learning

Problem Set #: ____

Please print out, fill in and include this cover sheet as the first page of your submission. We strongly recommend that you use this cover sheet, which will help us to get your graded homework back to you more quickly, as well as help us with tracking submissions.

Please mark the submission time clearly below. It is an honor code violation to write down the wrong time.

If you are submitting this homework late: Each student will have a total of **seven free late (calendar) days** to use for homeworks, project proposals and project milestones. Once these late days are exhausted, any assignments turned in late will be penalized 20% per late day. However, no assignment will be accepted **more than four days** after its due date, and late days cannot be used for the final project writeup. Each 24 hours or part thereof that a homework is late uses up one full late day.

On-campus (non-SCPD) students: Please either hand in the assignment at the beginning of class on Wednesday or leave it in the submission cabinet on the 1st floor of the Gates building, near/outside Gates 188 and 182.

Name: ____

SUNet ID: ____

Submission date: __________________ and time: ____________

Collaborators: ____

I understand and acknowledge CS229's Honor Code Policy (available online at http://cs229.stanford.edu/info.html)

Signature: ____

(For CS229 staff only)

Question	Score
1	
2	
3	
4	
5	
6	
Late Days	
Total	

CS 229, Autumn 2013
Problem Set #1 Solutions: Supervised Learning

Due in class (9:00am) on Wednesday, October 16.

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1. **[25 points] Logistic regression**

   (a) [10 points] Consider the log-likelihood function for logistic regression:

$$\ell(\theta) = \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)}))$$

Find the Hessian H of this function, and show that for any vector z, it holds true that

$$z^T H z \leq 0.$$

[Hint: You might want to start by showing the fact that $\sum_i \sum_j z_i x_i x_j z_j = (x^T z)^2 \geq 0$.]

Remark: This is one of the standard ways of showing that the matrix H is negative semi-definite, written "$H \leq 0$." This implies that ℓ is concave, and has no local maxima other than the global one.[1] If you have some other way of showing $H \leq 0$, you're also welcome to use your method instead of the one above.

Answer: (Note we do things in a slightly shorter way here; this solution does not use the hint.) Recall that we have $g'(z) = g(z)(1 - g(z))$, and thus for $h(x) = g(\theta^T x)$, we have $\frac{\partial h(x)}{\partial \theta_k} = h(x)(1 - h(x))x_k$. This latter fact is very useful to make the following derivations.

Remember we have shown in class:

$$\frac{\partial l(\theta)}{\partial \theta_k} = \sum_{i=1}^{m} (y^{(i)} - h(x^{(i)}))x_k^{(i)} \tag{1}$$

[1] If you haven't seen this result before, please feel encouraged to ask us about it during office hours.

$$\begin{aligned} H_{kl} &= \frac{\partial^2 l(\theta)}{\partial\theta_k \partial\theta_l} && (2)\\ &= \sum_{i=1}^{m} -\frac{\partial h(x^{(i)})}{\partial\theta_l} x_k^{(i)} && (3)\\ &= \sum_{i=1}^{m} -h(x^{(i)})(1-h(x^{(i)}))x_l^{(i)}x_k^{(i)} && (4)\\ & && (5) \end{aligned}$$

So we have for the hessian matrix H (using that for $X = xx^T$if and only if$X_{ij} = x_i x_j$):

$$\begin{aligned} H &= -\sum_{i=1}^{m} h(x^{(i)})(1-h(x^{(i)}))x^{(i)}x^{(i)T} && (6)\\ & && (7) \end{aligned}$$

And to prove H is negative semidefinite, we show $z^T Hz \le 0$ for all z.

$$\begin{aligned} z^T Hz &= -z^T \left(\sum_{i=1}^{m} h(x^{(i)})(1-h(x^{(i)}))x^{(i)}x^{(i)T} \right) z && (8)\\ &= -\sum_{i=1}^{m} h(x^{(i)})(1-h(x^{(i)}))z^T x^{(i)}x^{(i)T} z && (9)\\ &= -\sum_{i=1}^{m} h(x^{(i)})(1-h(x^{(i)}))(z^T x^{(i)})^2 && (10)\\ &\le 0 && (11) \end{aligned}$$

with the last inequality holding, since $0 \le h(x^{(i)}) \le 1$, which implies $h(x^{(i)})(1-h(x^{(i)})) \ge 0$, and $(z^T x^{(i)})^2) \ge 0$.

(b) [10 points] On the Leland system, the files `/afs/ir/class/cs229/ps/ps1/q1x.dat` and `/afs/ir/class/cs229/ps/ps1/q1y.dat` contain the inputs ($x^{(i)} \in \mathbb{R}^2$) and outputs ($y^{(i)} \in \{0,1\}$) respectively for a binary classification problem, with one training example per row. Implement[2] Newton's method for optimizing $\ell(\theta)$, 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? (Remember to include the intercept term.)

Answer: $\theta = (-2.6205, 0.7604, 1.1719)$ with the first entry corresponding to the intercept term.

```
%%%%%%%  hw1q1.m  %%%%%%%
load('q1x.dat');
load('q1y.dat');

q1x = [ones(size(q1x,1),1) q1x];
[theta, ll] = log_regression(q1x,q1y);

m=size(q1x,1);
```

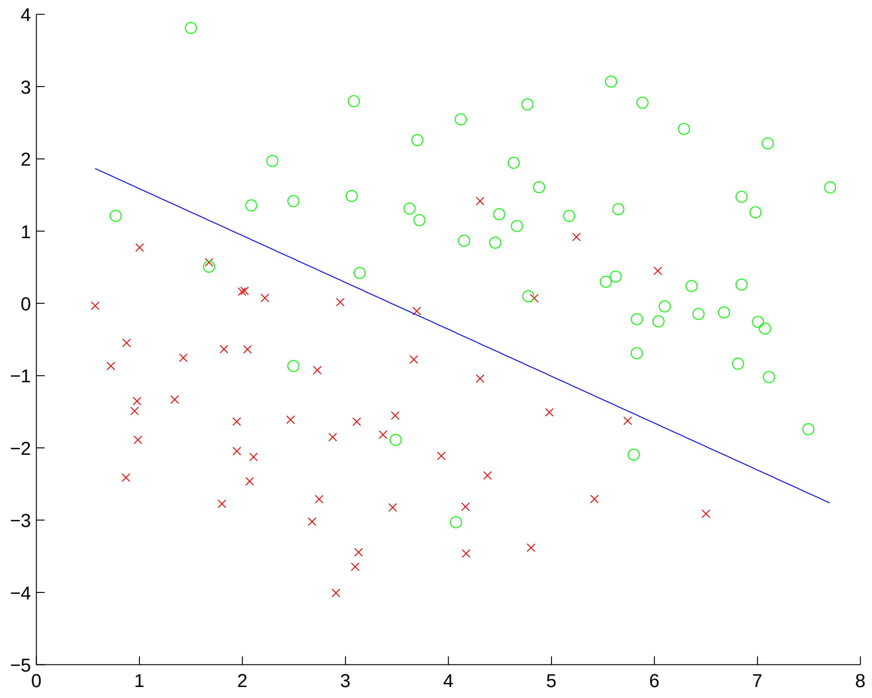
[2]Write your own version, and do not call a built-in library function.

```
figure; hold on;

for i=1:m
   if(q1y(i)==0)
      plot(q1x(i,2),q1x(i,3),'rx');
   else
      plot(q1x(i,2),q1x(i,3),'go');
   end
end

x = min(q1x(:,2)):.01:max(q1x(:,2));
y = -theta(1)/theta(3)-theta(2)/theta(3)*x;

plot(x,y);
xlabel('x1');
ylabel('x2');
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%% log_regression.m %%%%%%%

function [theta,ll] = log_regression(X,Y)

% rows of X are training samples
% rows of Y are corresponding 0/1 values

% newton raphson: theta = theta - inv(H)* grad;
% with H = hessian, grad = gradient

m = size(X,1);
n = size(X,2);

theta = zeros(n,1);

max_iters = 50;
for i=1:max_iters
   grad = zeros(n,1);
   ll(i)=0;
   H = zeros(n,n);
   for j=1:m
      hxj = sigmoid(X(j,:)*theta);
      grad = grad + X(j,:)'*(Y(j) - hxj);
      H = H - hxj*(1-hxj)*X(j,:)'*X(j,:);
      ll(i) = ll(i) + Y(j)*log(hxj) + (1-Y(j))*log(1-hxj);
   end
   theta = theta - inv(H)*grad;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%% sigmoid.m %%%%%%%%%%%%%%
```

```
function a = sigmoid(x)

a = 1./(1+exp(-x));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

(c) [5 points] 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 0). Also plot on the same figure the decision boundary fit by logistic regression. (I.e., this should be a straight line showing the boundary separating the region where $h(x) > 0.5$ from where $h(x) \leq 0.5$.)

Answer:



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

for an appropriate diagonal matrix W, and where X and $\vec{y}$ are as defined in class. State clearly what W is.

Answer: Let $W_{ii} = \frac{1}{2}w^{(i)}, W_{ij} = 0$ for $i \neq j$, let $\vec{z} = X\theta - \vec{y}$, i.e. $z_i = \theta^T x^{(i)} - y^{(i)}$. Then we have:

$$\begin{aligned}
(X\theta - \vec{y})^T W (X\theta - \vec{y}) &= \vec{z}^T W \vec{z} & (12)\\
&= \frac{1}{2}\sum_{i=1}^{m} w^{(i)} z_i^2 & (13)\\
&= \frac{1}{2}\sum_{i=1}^{m} w^{(i)} (\theta^T x^{(i)} - y^{(i)})^2 & (14)\\
&= J(\theta) & (15)
\end{aligned}$$

(b) [7 points] If all the $w^{(i)}$'s equal 1, then we saw in class that the normal equation is

$$X^T X\theta = X^T \vec{y},$$

and that the value of θ that minimizes $J(\theta)$ is given by $(X^T X)^{-1} X^T \vec{y}$. 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 of X, W and $\vec{y}$.

Answer:

$$\nabla_\theta J(\theta) = \nabla_\theta(\theta^T X^T W X\theta + \vec{y}^T W \vec{y} - 2\vec{y}^T W X\theta) = 2(X^T W X\theta - X^T W \vec{y}), \qquad (16)$$

so we have $\nabla_\theta J(\theta) = 0$ if and only if

$$X^T W X\theta = X^T W \vec{y} \qquad (17)$$

These are the normal equations, from which we can get a closed form formula for θ.

$$\theta = (X^T W X)^{-1} X^T W \vec{y} \qquad (18)$$

(c) [6 points] Suppose we have a training set $\{(x^{(i)}, y^{(i)});\ i = 1\dots, m\}$ 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.

Answer:

$$\begin{aligned}
\arg\max_\theta \prod_{i=1}^m p(y^{(i)}|x^{(i)};\theta) &= \arg\max_\theta \sum_{i=1}^m \log p(y^{(i)}|x^{(i)};\theta) && (19)\\
&= \arg\max_\theta \sum_{i=1}^m \left(\log\frac{1}{\sqrt{2\pi}\sigma^{(i)}} - \frac{(y^{(i)}-\theta^T x^{(i)})^2}{2(\sigma^{(i)})^2}\right) && (20)\\
&= \arg\max_\theta -\sum_{i=1}^m \frac{(y^{(i)}-\theta^T x^{(i)})^2}{2(\sigma^{(i)})^2} && (21)\\
&= \arg\min_\theta \frac{1}{2}\sum_{i=1}^m \frac{1}{(\sigma^{(i)})^2}(y^{(i)}-\theta^T x^{(i)})^2 && (22)\\
&= \arg\min_\theta \frac{1}{2}\sum_{i=1}^m w^{(i)}(y^{(i)}-\theta^T x^{(i)})^2 && (23)
\end{aligned}$$

where in the last step, we substituted: $w^{(i)} = \frac{1}{(\sigma^{(i)})^2}$ to get the linear regression form.

(d) [12 points] On the Leland computer system, the files `/afs/ir/class/cs229/ps/ps1/q2x.dat` and `/afs/ir/class/cs229/ps/ps1/q2y.dat` contain the inputs ($x^{(i)}$) and outputs ($y^{(i)}$) for a regression problem, with one training example per row.

i. [2 points] Implement (unweighted) linear regression ($y = \theta^T x$) on this dataset (using the normal equations), and plot on the same figure the data and the straight line resulting from your fit. (Remember to include the intercept term.)

ii. [7 points] Implement locally weighted linear regression on this dataset (using the weighted normal equations you derived in part (b)), and plot on the same figure the data and the 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 a bandwidth parameter $\tau = 0.8$. (Again, remember to include the intercept term.)

iii. [3 points] Repeat (ii) four times, with $\tau = 0.1, 0.3, 2$ and 10. Comment **briefly** on what happens to the fit when τ is too small or too large.

Answer: Below is the code for all 3 parts of question 2d:

```
%%%%%%% hw1q2d %%%%%%%%

load('q2x.dat');
load('q2y.dat');

x = [ones(size(q2x,1),1) q2x];
y = q2y;

%% linear regression
theta = pinv(x'*x)*x'*y;

figure;
```

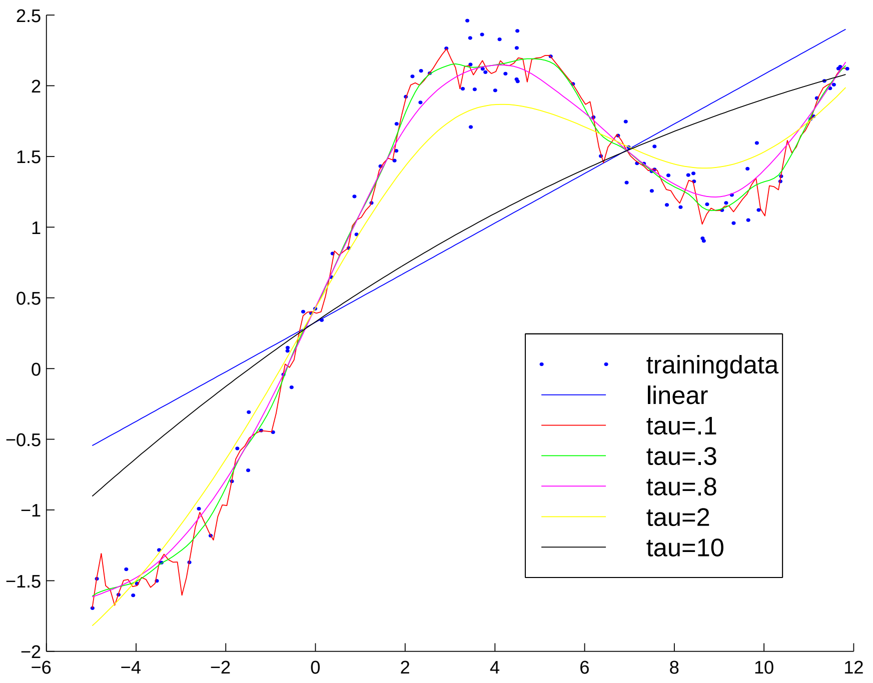
```
hold on;
plot(x(:,2),y,'.b');
regr_line_x = min(x(:,2)):.1:max(x(:,2));
regr_line_y = theta(2)*regr_line_x + theta(1);
plot(regr_line_x,regr_line_y,'b');




%% locally weighted linear regression

taus = [.1 .3 .8 2 10];
colors = ['r' 'g' 'm' 'y' 'k'];
m = size(q2x,1);

for i=1:size(taus,2)
   tau=taus(i);
   for k=1:size(regr_line_x,2)
      W = zeros(m,m);
      for l=1:m
         W(l,l)=exp(-(regr_line_x(k)-x(l,2))^2/(2*tau^2));
      end
      theta = pinv(x'*W*x)*x'*W*y;
      regr_line_y(k) = theta(2)*regr_line_x(k) + theta(1);
   end
   plot(regr_line_x,regr_line_y,colors(i));
end
legend('trainingdata','linear','tau=.1','tau=.3',...
    'tau=.8','tau=2','tau=10')
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```



(Plotted in color where available.)

For small bandwidth parameter τ, the fitting is dominated by the closest by training samples. The smaller the bandwidth, the less training samples that are actually taken into account when doing the regression, and the regression results thus become very susceptible to noise in those few training samples. For larger τ, we have enough training samples to reliably fit straight lines, unfortunately a straight line is not the right model for these data, so we also get a bad fit for large bandwidths.

3. **[18 points] Poisson regression and the exponential family**

   (a) [5 points] 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 $a(\eta)$.

Answer: Rewrite the distribution function as:

$$\begin{aligned} p(y;\lambda) &= \frac{e^{-\lambda}e^{y\log\lambda}}{y!} \\ &= \frac{1}{y!}\exp(y\log\lambda - \lambda) \end{aligned}$$

Comparing with the standard form for the exponential family:

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

(b) [3 points] 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.)

Answer: The canonical response function for the GLM model will be:

$$\begin{aligned} g(\eta) &= E[y;\eta] \\ &= \lambda \\ &= e^{\eta} \end{aligned}$$

(c) [10 points] For a training set $\{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$, 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.

Answer: The log-likelihood of an example $(x^{(i)}, y^{(i)})$ is defined as $\ell(\theta) = \log p(y^{(i)}|x^{(i)};\theta)$. To derive the stochastic gradient ascent rule, use the results in part (a) and the standard GLM assumption that $\eta = \theta^T x$.

$$\begin{aligned} \frac{\partial \ell(\theta)}{\partial \theta_j} &= \frac{\partial \log p(y^{(i)}|x^{(i)};\theta)}{\partial \theta_j} \\ &= \frac{\partial \log \left(\frac{1}{y^{(i)}!} \exp(\eta^T y^{(i)} - e^{\eta})\right)}{\partial \theta_j} \\ &= \frac{\partial \log \left(\exp((\theta^T x^{(i)})^T y^{(i)} - e^{\theta^T x^{(i)}})\right)}{\partial \theta_j} + \frac{\partial \log \left(\frac{1}{y^{(i)}!}\right)}{\partial \theta_j} \\ &= \frac{\partial \left((\theta^T x^{(i)})^T y^{(i)} - e^{\theta^T x^{(i)}}\right)}{\partial \theta_j} \\ &= \frac{\partial \left((\sum_k \theta_k x_k^{(i)}) y^{(i)} - e^{\sum_k \theta_k x_k^{(i)}}\right)}{\partial \theta_j} \\ &= x_j^{(i)} y^{(i)} - e^{\sum_k \theta_k x_k^{(i)}} x_j^{(i)} \\ &= (y^{(i)} - e^{\theta^T x^{(i)}}) x_j^{(i)} \end{aligned}$$

Thus the stochastic gradient ascent update rule should be:

$$\theta_j := \theta_j + \alpha \frac{\partial \ell(\theta)}{\partial \theta_j}$$

which reduces here to:

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

(d) **[5 extra credit points]** Consider using GLM with a response variable from any member of the exponential family in which $T(y) = y$, and the canonical response function for the family. Show that stochastic gradient ascent on the log-likelihood $\log p(\vec{y}|X, \theta)$ results in the update rule $\theta_i := \theta_i - \alpha(h(x) - y)x_i$.

Answer: As in the previous part, consider the derivative of the likelihood of a training example (x, y) with respect to the parameter θ_j:

$$\begin{aligned}
\frac{\partial \ell(\theta)}{\partial \theta_j} &= \frac{\partial \log p(y|x;\theta)}{\partial \theta_j} \\
&= \frac{\partial \log \left(b(y)\exp(\eta^T y - a(\eta))\right)}{\partial \theta_j} \\
&= \frac{\partial \left(\eta^T y - a(\eta))\right)}{\partial \theta_j} \\
&= x_j y - \frac{\partial a(\eta)}{\partial \eta} x_j \\
&= \left(y - \frac{\partial a(\eta)}{\partial \eta}\right) x_j
\end{aligned}$$

Thus, it only remains to show that $\frac{\partial a(\eta)}{\partial \eta} = h(x) = E[y|x;\theta]$. To prove this consider the fact that $p(y|x;\theta)$ is a probability distribution and must thus sum to 1.

$$\begin{aligned}
\int_y p(y|x;\theta)dy &= 1 \\
\int_y b(y)\exp(\eta^T y - a(\eta))dy &= 1 \\
\int_y b(y)\exp(\eta^T y)dy &= \exp(a(\eta))
\end{aligned}$$

Differentiating both sides with respect to η:

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

where the last step follows from the definition of the (conditional) expectation of a random variable. Substituting this into the expression for $\frac{\partial \ell(\theta)}{\partial \theta_j}$ gives the required gradient ascent update rule.

4. **[15 points] Gaussian discriminant analysis**

Suppose we are given a dataset $\{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$ consisting of m independent examples, where $x^{(i)} \in \mathbb{R}^n$ are n-dimensional vectors, and $y^{(i)} \in \{0, 1\}$. We will model the joint distribution of (x, y) according to:

$$\begin{aligned} p(y) &= \phi^y (1-\phi)^{1-y} \\ p(x|y=0) &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1} (x-\mu_0)\right) \\ p(x|y=1) &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1} (x-\mu_1)\right) \end{aligned}$$

Here, the parameters of our model are ϕ, Σ, μ_0 and μ_1. (Note that while there're two different mean vectors μ_0 and μ_1, there's only one covariance matrix Σ.)

(a) [5 points] Suppose we have already fit ϕ, Σ, μ_0 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

$$p(y=1|x; \phi, \Sigma, \mu_0, \mu_1) = \frac{1}{1+\exp(-\theta^T x)},$$

where θ is some appropriate function of $\phi, \Sigma, \mu_0, \mu_1$. (Note: To get your answer into the form above, for this part of the problem only, you may have to redefine the $x^{(i)}$'s to be $n+1$-dimensional vectors by adding the extra coordinate $x_0^{(i)} = 1$, like we did in class.)

Answer: Since the given formulae are conditioned on y, use Bayes rule to get:

$$\begin{aligned} p(y=1|x;\phi,\Sigma,\mu_0,\mu_1) &= \frac{p(x|y=1;\phi,\Sigma,\mu_0,\mu_1)p(y=1;\phi,\Sigma,\mu_0,\mu_1)}{p(x;\phi,\Sigma,\mu_0,\mu_1)} \\ &= \frac{p(x|y=1;\ldots)p(y=1;\ldots)}{p(x|y=1;\ldots)p(y=1;\ldots)+p(x|y=0;\ldots)p(y=0;\ldots)} \\ &= \frac{\exp\left(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)\phi}{\exp\left(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)\phi + \exp\left(-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)\right)(1-\phi)} \\ &= \frac{1}{1+\frac{1-\phi}{\phi}\exp\left(-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)+\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)} \\ &= \frac{1}{1+\exp\left(\log(\frac{1-\phi}{\phi})-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)+\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)} \\ &= \frac{1}{1+\exp\left(-\frac{1}{2}\left(-2\mu_0^T\Sigma^{-1}x+\mu_0^T\Sigma^{-1}\mu_0+2\mu_1^T\Sigma^{-1}x-\mu_1^T\Sigma^{-1}\mu_1\right)+\log(\frac{1-\phi}{\phi})\right)} \end{aligned}$$

where we have simplified the denominator in the penultimate step by expansion, i.e.,

$$\begin{aligned} &-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)+\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1) \\ &= -\frac{1}{2}\left(x^T\Sigma^{-1}x-\mu_0^T\Sigma^{-1}x-x^T\Sigma^{-1}\mu_0+\mu_0^T\Sigma^{-1}\mu_0-x^T\Sigma^{-1}x+\mu_1^T\Sigma^{-1}x+x^T\Sigma^{-1}\mu_1-\mu_1^T\Sigma^{-1}\mu_1\right) \\ &= -\frac{1}{2}\left(\mu_0^T\Sigma^{-1}x-(x^T\Sigma^{-1}\mu_0)^T+\mu_0^T\Sigma^{-1}\mu_0+\mu_1^T\Sigma^{-1}x+(x^T\Sigma^{-1}\mu_1)^T-\mu_1^T\Sigma^{-1}\mu_1\right) \end{aligned}$$

Recall that the question was to find θ for $\exp(-\theta^T x)$, after adding a constant intercept term $x_0 = 1$, we have θ equal to:

$$\begin{bmatrix} \frac{1}{2}(\mu_0^T\Sigma^{-1}\mu_0 - \mu_1^T\Sigma^{-1}\mu_1) - \log(\frac{1-\phi}{\phi}) \\ \Sigma^{-1}\mu_1 - \Sigma^{-1}\mu_0 \end{bmatrix}$$

(b) [10 points] 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 $|\Sigma| = \sigma^2$. Given the dataset, we claim that the maximum likelihood estimates of the parameters are given by

$$\begin{aligned} \phi &= \frac{1}{m}\sum_{i=1}^m 1\{y^{(i)} = 1\} \\ \mu_0 &= \frac{\sum_{i=1}^m 1\{y^{(i)} = 0\}x^{(i)}}{\sum_{i=1}^m 1\{y^{(i)} = 0\}} \\ \mu_1 &= \frac{\sum_{i=1}^m 1\{y^{(i)} = 1\}x^{(i)}}{\sum_{i=1}^m 1\{y^{(i)} = 1\}} \\ \Sigma &= \frac{1}{m}\sum_{i=1}^m (x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T \end{aligned}$$

The log-likelihood of the data is

$$\begin{aligned} \ell(\phi, \mu_0, \mu_1, \Sigma) &= \log\prod_{i=1}^m p(x^{(i)}, y^{(i)}; \phi, \mu_0, \mu_1, \Sigma) \\ &= \log\prod_{i=1}^m p(x^{(i)}|y^{(i)}; \mu_0, \mu_1, \Sigma)p(y^{(i)}; \phi). \end{aligned}$$

By maximizing ℓ with respect to the four parameters, prove that the maximum likelihood estimates of ϕ, μ_0, μ_1, and Σ are indeed as given in the formulas above. (You may assume that there is at least one positive and one negative example, so that the denominators in the definitions of μ_0 and μ_1 above are non-zero.)

Answer: The derivation follows from the more general one for the next part.

(c) **[5 extra credit points]** Without assuming that $n = 1$, show that the maximum likelihood estimates of ϕ, μ_0, μ_1, and Σ are as given in the formulas in part (b). [Note: If you're fairly sure that you have the answer to this part right, you don't have to do part (b), since that's just a special case.]

Answer: First, derive the expression for the log-likelihood of the training data:

$$\begin{aligned} \ell(\phi, \mu_0, \mu_1, \Sigma) &= \log\prod_{i=1}^m p(x^{(i)}|y^{(i)}; \mu_0, \mu_1, \Sigma)p(y^{(i)}; \phi) \\ &= \sum_{i=1}^m \log p(x^{(i)}|y^{(i)}; \mu_0, \mu_1, \Sigma) + \sum_{i=1}^m \log p(y^{(i)}; \phi) \\ &\simeq \sum_{i=1}^m \big[\frac{1}{2}\log\frac{1}{|\Sigma|} - \frac{1}{2}(x^{(i)} - \mu_{y^{(i)}})^T\Sigma^{-1}(x^{(i)} - \mu_{y^{(i)}}) + y^{(i)}\log\phi + (1 - y^{(i)})\log(1-\phi)\big] \end{aligned}$$

where constant terms indepedent of the parameters have been ignored in the last expression.

Now, the likelihood is maximized by setting the derivative (or gradient) with respect to each of the parameters to zero.

$$\begin{aligned}
\frac{\partial \ell}{\partial \phi} &= \sum_{i=1}^{m} [\frac{y^{(i)}}{\phi} - \frac{1-y^{(i)}}{1-\phi}] \\
&= \frac{\sum_{i=1}^{m} 1\{y^{(i)}=1\}}{\phi} - \frac{m - \sum_{i=1}^{m} 1\{y^{(i)}=1\}}{1-\phi}
\end{aligned}$$

Setting this equal to zero and solving for ϕ gives the maximum likelihood estimate.

For μ_0, take the gradient of the log-likelihood, and then use the same kinds of tricks as were used to analytically solve the linear regression problem.

$$\begin{aligned}
\nabla_{\mu_0} \ell &= -\frac{1}{2} \sum_{i:y^{(i)}=0} \nabla_{\mu_0} (x^{(i)} - \mu_0)^T \Sigma^{-1} (x^{(i)} - \mu_0) \\
&= -\frac{1}{2} \sum_{i:y^{(i)}=0} \nabla_{\mu_0} \left[\mu_0^T \Sigma^{-1} \mu_0 - {x^{(i)}}^T \Sigma^{-1} \mu_0 - \mu_0^T \Sigma^{-1} x^{(i)}\right] \\
&= -\frac{1}{2} \sum_{i:y^{(i)}=0} \nabla_{\mu_0} tr \left[\mu_0^T \Sigma^{-1} \mu_0 - {x^{(i)}}^T \Sigma^{-1} \mu_0 - \mu_0^T \Sigma^{-1} x^{(i)}\right] \\
&= -\frac{1}{2} \sum_{i:y^{(i)}=0} \left[2\Sigma^{-1}\mu_0 - 2\Sigma^{-1} x^{(i)}\right]
\end{aligned}$$

The last step uses matrix calculus identities (specifically, those given in page 8 of the lecture notes), and also the fact that Σ (and thus Σ^{-1}) is symmetric.

Setting this gradient to zero gives the maximum likelihood estimate for μ_0. The derivation for μ_1 is similar to the one above.

For Σ, we find the gradient with respect to $S = \Sigma^{-1}$ rather than Σ just to simplify the derivation (note that $|S| = \frac{1}{|\Sigma|}$). You should convince yourself that the maximum likelihood estimate S_m found in this way would correspond to the actual maximum likelihood estimate Σ_m as $S_m^{-1} = \Sigma_m$.

$$\begin{aligned}
\nabla_S \ell &= \sum_{i=1}^{m} \nabla_S \big[\frac{1}{2} \log |S| - \frac{1}{2} \underbrace{(x^{(i)} - \mu_{y^{(i)}})^T}_{b_i^T} S \underbrace{(x^{(i)} - \mu_{y^{(i)}})}_{b_i}\big] \\
&= \sum_{i=1}^{m} \big[\frac{1}{2|S|} \nabla_S |S| - \frac{1}{2} \nabla_S b_i^T S b_i\big]
\end{aligned}$$

But, we have the following identities:

$$\nabla_S |S| = |S| (S^{-1})^T$$

$$\nabla_S b_i^T S b_i = \nabla_S tr\left(b_i^T S b_i\right) = \nabla_S tr\left(S b_i b_i^T\right) = b_i b_i^T$$

In the above, we again used matrix calculus identities, and also the commutatitivity of the trace operator for square matrices. Putting these into the original equation, we get:

$$\begin{aligned}\nabla_S \ell &= \sum_{i=1}^{m} \big[\frac{1}{2}S^{-1} - \frac{1}{2}b_i b_i^T\big] \\ &= \frac{1}{2}\sum_{i=1}^{m}\big[\Sigma - b_i b_i^T\big]\end{aligned}$$

Setting this to zero gives the required maximum likelihood estimate for Σ.

5. **[12 points] Linear invariance of optimization 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 $x^{(0)} = \vec{0}$. When the algorithm is run, it will produce a value of $x \in \mathbb{R}^n$ for each iteration: $x^{(1)}, x^{(2)}, \ldots$.

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

(a) [9 points] Show that Newton's method (applied to find the minimum of a function) is invariant to linear reparameterizations. Note that since $z^{(0)} = \vec{0} = A^{-1}x^{(0)}$, it is sufficient to show that if Newton's method applied to $f(x)$ updates $x^{(i)}$ to $x^{(i+1)}$, then Newton's method applied to $g(z)$ will update $z^{(i)} = A^{-1}x^{(i)}$ to $z^{(i+1)} = A^{-1}x^{(i+1)}$.[3]

Answer: Let $g(z) = f(Az)$. We need to find $\nabla_z g(z)$ and its Hessian $\nabla_z^2 g(z)$.

By the chain rule:

$$\begin{aligned}\frac{\partial g(z)}{\partial z_i} &= \sum_{k=1}^{n}\frac{\partial f(Az)}{\partial (Az)_k}\frac{\partial (Az)_k}{\partial z_i} && (24)\\ &= \sum_{k=1}^{n}\frac{\partial f(Az)}{\partial (Az)_k}A_{ki} && (25)\\ &= \sum_{k=1}^{n}\frac{\partial f(Az)}{\partial x_k}A_{ki} && (26)\end{aligned}$$

Notice that the above is the same as :

$$\frac{\partial g(z)}{\partial z_i} = A_{\bullet i}^{\top}\nabla_x f(Az) \qquad (27)$$

where $A_{\bullet i}$ is the i'th column of A. Then,

$$\nabla_z g(z) = A^{\top}\nabla_x f(Az) \qquad (28)$$

[3]Note that for this problem, you must explicitly prove any matrix calculus identities that you wish to use that are not given in the lecture notes.

where $\nabla_x f(Az)$ is $\nabla_x f(\cdot)$ evaluated at Az.

Now we want to find the Hessian $\nabla_z^2 g(z)$.

$$\begin{aligned}\frac{\partial^2 g(z)}{\partial z_i \partial z_j} &= \frac{\partial}{\partial z_j}\sum_{k=1}^{n}\frac{\partial f(Az)}{\partial (Az)_k}A_{ki} && (29)\\ &= \sum_l\sum_k \frac{\partial^2 f(Az)}{\partial x_l \partial x_k}A_{ki}A_{lj} && (30)\end{aligned}$$

If we let $H_f(y)$ denote the Hessian of $f(\cdot)$ evaluated at some point y, and let $H_g(y)$ be the Hessian of $g(\cdot)$ evaluated at some point y, we have from the previous equation that:

$$H_g(z) = A^\top H_f(Az)A \quad (31)$$

We can now put this together and find the update rule for Newton's method on the function $f(Ax)$:

$$\begin{aligned}z^{(i+1)} &= z^{(i)} - H_g(z^{(i)})^{-1}\nabla_z g(z^{(i)}) && (32)\\ &= z^{(i)} - (A^\top H_f(Az^{(i)})A)^{-1}A^\top \nabla_x f(Az^{(i)}) && (33)\\ &= z^{(i)} - A^{-1}H_f(Az^{(i)})^{-1}(A^\top)^{-1}A^\top \nabla_x f(Az^{(i)}) && (34)\\ &= z^{(i)} - A^{-1}H_f(Az^{(i)})^{-1}\nabla_x f(Az^{(i)}) && (35)\end{aligned}$$

Now we have the update rule for $z^{(i+1)}$, we just need to verify that $z^{(i+1)} = A^{-1}x^{(i+1)}$ or equivalently that $Az^{(i+1)} = x^{(i+1)}$. From Eqn. (**??**) we have

$$\begin{aligned}Az^{(i+1)} &= A\left(z^{(i)} - A^{-1}H_f(Az^{(i)})^{-1}\nabla_x f(Az^{(i)})\right) && (36)\\ &= Az^{(i)} - H_f(Az^{(i)})^{-1}\nabla_x f(Az^{(i)}) && (37)\\ &= x^{(i)} - H_f(x^{(i)})^{-1}\nabla_x f(x^{(i)}) && (38)\\ &= x^{(i+1)}, && (39)\end{aligned}$$

where we used in order: Eqn. (**??**); rewriting terms; the inductive assumption $x^{(i)} = Az^{(i)}$; the update rule $x^{(i+1)} = x^{(i)} - H_f(x^{(i)})^{-1}\nabla_x f(x^{(i)})$.

(b) [3 points] Is gradient descent invariant to linear reparameterizations? Justify your answer.

Answer:

No. Using the notation from above, gradient descent on $g(z)$ results in the following update rule:

$$z^{(i+1)} = z^{(i)} - \alpha A^\top \nabla_x f(Az^{(i)}). \quad (40)$$

The update rule for $x^{(i+1)}$ is given by

$$x^{(i+1)} = x^{(i)} - \alpha \nabla_x f(x^{(i)}). \quad (41)$$

The invariance holds if and only if $x^{(i+1)} = Az^{(i+1)}$ given $x^{(i)} = Az^{(i)}$. However we have

$$\begin{aligned} Az^{(i+1)} &= Az^{(i)} - \alpha AA^\top \nabla_x f(Az^{(i)}) &(42)\\ &= x^{(i)} - \alpha AA^\top \nabla_x f(x^{(i)}). &(43)\end{aligned}$$

The two expressions in Eqn. (??) and Eqn. (??) are not necessarily equal ($AA^T = I$ requires that A be an orthogonal matrix), and thus gradient descent is not invariant to linear reparameterizations.

Reminder: Please include in your submission a printout of your code and figures for the programming questions.

CS 229, Autumn 2013
Problem Set #2: Naive Bayes, SVMs, and Theory

Due in class (9:00am) on Wednesday, October 30.

Notes: (1) These questions require thought, but do not require long answers. Please be as concise as possible. (2) If you have a question about this homework, we encourage you to post your question on our Piazza forum, at `https://piazza.com/stanford/fall2013/cs229`. (3) If you missed the first lecture or are unfamiliar with the collaboration or honor code policy, please read the policy on Handout #1 (available from the course website) before starting work. (4) For problems that require programming, please include in your submission a printout of your code (with comments) and any figures that you are asked to plot. (5) If you are an on-campus (non-SCPD) student, please print, fill out, and include a copy of the cover sheet (enclosed as the final page of this document), and include the cover sheet as the first page of your submission.

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If you are scanning your document by cellphone, please check the Piazza forum for recommended cellphone scanning apps and best practices.

1. **[15 points] Constructing kernels**

   In class, we saw that by choosing a kernel $K(x,z) = \phi(x)^T\phi(z)$, we can implicitly map data to a high dimensional space, and have the SVM algorithm work in that space. One way to generate kernels is to explicitly define the mapping ϕ to a higher dimensional space, and then work out the corresponding K.

   However in this question we are interested in direct construction of kernels. I.e., suppose we have a function $K(x,z)$ that we think gives an appropriate similarity measure for our learning problem, and we are considering plugging K into the SVM as the kernel function. However for $K(x,z)$ to be a valid kernel, it must correspond to an inner product in some higher dimensional space resulting from some feature mapping ϕ. Mercer's theorem tells us that $K(x,z)$ is a (Mercer) kernel if and only if for any finite set $\{x^{(1)},\dots,x^{(m)}\}$, the matrix K is symmetric and positive semidefinite, where the square matrix $K \in \mathbb{R}^{m\times m}$ is given by $K_{ij} = K(x^{(i)}, x^{(j)})$.

   Now here comes the question: Let K_1, K_2 be kernels over $\mathbb{R}^n \times \mathbb{R}^n$, let $a \in \mathbb{R}^+$ be a positive real number, let $f : \mathbb{R}^n \mapsto \mathbb{R}$ be a real-valued function, let $\phi : \mathbb{R}^n \to \mathbb{R}^d$ be a function mapping from $\mathbb{R}^n$ to $\mathbb{R}^d$, let K_3 be a kernel over $\mathbb{R}^d \times \mathbb{R}^d$, and let $p(x)$ a polynomial over x with *positive* coefficients.

   For each of the functions K below, state whether it is necessarily a kernel. If you think it is, prove it; if you think it isn't, give a counter-example.

   (a) $K(x,z) = K_1(x,z) + K_2(x,z)$

   (b) $K(x,z) = K_1(x,z) - K_2(x,z)$

   (c) $K(x,z) = aK_1(x,z)$

(d) $K(x, z) = -aK_1(x, z)$

(e) $K(x, z) = K_1(x, z)K_2(x, z)$

(f) $K(x, z) = f(x)f(z)$

(g) $K(x, z) = K_3(\phi(x), \phi(z))$

(h) $K(x, z) = p(K_1(x, z))$

[Hint: For part (e), the answer is that the K there *is* indeed a kernel. You still have to prove it, though. (This one may be harder than the rest.) This result may also be useful for another part of the problem.]

2. **[15 points] Kernelizing the Perceptron**

Let there be a binary classification problem with $y \in \{0, 1\}$. The perceptron uses hypotheses of the form $h_\theta(x) = g(\theta^T x)$, where $g(z) = \mathbf{1}\{z \geq 0\}$. In this problem we will consider a stochastic gradient descent-like implementation of the perceptron algorithm where each update to the parameters θ is made using only one training example. However, unlike stochastic gradient descent, the perceptron algorithm will only make one pass through the entire training set. The update rule for this version of the perceptron algorithm is given by

$$\theta^{(i+1)} := \theta^{(i)} + \alpha[y^{(i+1)} - h_{\theta^{(i)}}(x^{(i+1)})]x^{(i+1)}$$

where $\theta^{(i)}$ is the value of the parameters after the algorithm has seen the first i training examples. Prior to seeing any training examples, $\theta^{(0)}$ is initialized to $\vec{0}$.

Let K be a Mercer kernel corresponding to some very high-dimensional feature mapping ϕ. Suppose ϕ is so high-dimensional (say, ∞-dimensional) that it's infeasible to ever represent $\phi(x)$ explicitly. Describe how you would apply the "kernel trick" to the perceptron to make it work in the high-dimensional feature space ϕ, but without ever explicitly computing $\phi(x)$. [Note: You don't have to worry about the intercept term. If you like, think of ϕ as having the property that $\phi_0(x) = 1$ so that this is taken care of.] Your description should specify

(a) How you will (implicitly) represent the high-dimensional parameter vector $\theta^{(i)}$, including how the initial value $\theta^{(0)} = \vec{0}$ is represented (note that $\theta^{(i)}$ is now a vector whose dimension is the same as the feature vectors $\phi(x)$);

(b) How you will efficiently make a prediction on a new input $x^{(i+1)}$. I.e., how you will compute $h_{\theta^{(i)}}(x^{(i+1)}) = g({\theta^{(i)}}^T \phi(x^{(i+1)}))$, using your representation of $\theta^{(i)}$; and

(c) How you will modify the update rule given above to perform an update to θ on a new training example $(x^{(i+1)}, y^{(i+1)})$; i.e., using the update rule corresponding to the feature mapping ϕ:

$$\theta^{(i+1)} := \theta^{(i)} + \alpha[y^{(i+1)} - h_{\theta^{(i)}}(\phi(x^{(i+1)}))]\phi(x^{(i+1)})$$

[Note: If you prefer, you are also welcome to do this problem using the convention of labels $y \in \{-1, 1\}$, and $g(z) = \text{sign}(z) = 1$ if $z \geq 0$, -1 otherwise.]

3. **[30 points] Spam classification**

In this problem, we will use the naive Bayes algorithm and an SVM to build a spam classifier.

In recent years, spam on electronic newsgroups has been an increasing problem. Here, we'll build a classifier to distinguish between "real" newsgroup messages, and spam messages.

For this experiment, we obtained a set of spam emails, and a set of genuine newsgroup messages.[1] Using only the subject line and body of each message, we'll learn to distinguish between the spam and non-spam.

All the files for the problem are in `/afs/ir/class/cs229/ps/ps2/`. **Note: Please do not circulate this data outside this class.** In order to get the text emails into a form usable by naive Bayes, we've already done some preprocessing on the messages. You can look at two sample spam emails in the files `spam_sample_original*`, and their preprocessed forms in the files `spam_sample_preprocessed*`. The first line in the preprocessed format is just the label and is not part of the message. The preprocessing ensures that only the message body and subject remain in the dataset; email addresses (EMAILADDR), web addresses (HTTPADDR), currency (DOLLAR) and numbers (NUMBER) were also replaced by the special tokens to allow them to be considered properly in the classification process. (In this problem, we'll going to call the features "tokens" rather than "words," since some of the features will correspond to special values like EMAILADDR. You don't have to worry about the distinction.) The files `news_sample_original` and `news_sample_preprocessed` also give an example of a non-spam mail.

The work to extract feature vectors out of the documents has also been done for you, so you can just load in the design matrices (called document-word matrices in text classification) containing all the data. In a document-word matrix, the i^{th} row represents the i^{th} document/email, and the j^{th} column represents the j^{th} distinct token. Thus, the (i, j)-entry of this matrix represents the number of occurrences of the j^{th} token in the i^{th} document.

For this problem, we've chosen as our set of tokens considered (that is, as our vocabulary) only the medium frequency tokens. The intuition is that tokens that occur too often or too rarely do not have much classification value. (Examples tokens that occur very often are words like "the," "and," and "of," which occur in so many emails and are sufficiently content-free that they aren't worth modeling.) Also, words were stemmed using a standard stemming algorithm; basically, this means that "price," "prices" and "priced" have all been replaced with "price," so that they can be treated as the same word. For a list of the tokens used, see the file `TOKENS_LIST`.

Since the document-word matrix is extremely sparse (has lots of zero entries), we have stored it in our own efficient format to save space. You don't have to worry about this format.[2] The file `readMatrix.m` provides the `readMatrix` function that reads in the document-word matrix and the correct class labels for the various documents. Code in `nb_train.m` and `nb_test.m` shows how `readMatrix` should be called. The documentation at the top of these two files will tell you all you need to know about the setup.

(a) Implement a naive Bayes classifier for spam classification, using the multinomial event model and Laplace smoothing.

You should use the code outline provided in `nb_train.m` to train your parameters, and then use these parameters to classify the test set data by filling in the code in `nb_test.m`. You may assume that any parameters computed in `nb_train.m` are in memory when `nb_test.m` is executed, and do not need to be recomputed (i.e., that `nb_test.m` is executed immediately after `nb_train.m`) [3].

[1] Thanks to Christian Shelton for providing the spam email. The non-spam messages are from the 20 newsgroups data at http://www-2.cs.cmu.edu/afs/cs.cmu.edu/project/theo-20/www/data/news20.html .

[2] Unless you're not using Matlab/Octave, in which case feel free to ask us about it.

[3] Matlab note: If a .m file doesn't begin with a function declaration, the file is a script. Variables in a script are put into the global namespace, unlike with functions.

Train your parameters using the document-word matrix in `MATRIX.TRAIN`, and then report the test set error on `MATRIX.TEST`.

Remark. If you implement naive Bayes the straightforward way, you'll find that the computed $p(x|y) = \prod_i p(x_i|y)$ often equals zero. This is because $p(x|y)$, which is the product of many numbers less than one, is a very small number. The standard computer representation of real numbers cannot handle numbers that are too small, and instead rounds them off to zero. (This is called "underflow.") You'll have to find a way to compute naive Bayes' predicted class labels without explicitly representing very small numbers such as $p(x|y)$. [Hint: Think about using logarithms.]

(b) Intuitively, some tokens may be particularly indicative of an email being in a particular class. We can try to get an informal sense of how indicative token i is for the SPAM class by looking at:

$$\log \frac{p(x_j = i|y = 1)}{p(x_j = i|y = 0)} = \log \left(\frac{P(\text{token } i|\text{email is SPAM})}{P(\text{token } i|\text{email is NOTSPAM})} \right).$$

Using the parameters fit in part (a), find the 5 tokens that are most indicative of the SPAM class (i.e., have the highest positive value on the measure above). The numbered list of tokens in the file `TOKENS_LIST` should be useful for identifying the words/tokens.

(c) Repeat part (a), but with training sets of size ranging from 50, 100, 200, . . . , up to 1400, by using the files `MATRIX.TRAIN.*`. Plot the test error each time (use `MATRIX.TEST` as the test data) to obtain a learning curve (test set error vs. training set size). You may need to change the call to `readMatrix` in `nb_train.m` to read the correct file each time. Which training-set size gives the best test set error?

(d) Train an SVM on this dataset using the LIBLINEAR SVM library, available for download from http://www.csie.ntu.edu.tw/~cjlin/liblinear/. This implements an SVM using a linear kernel. Like the Naive Bayes implementation, an outline for your code is provided in `svm_train.m` and `svm_test.m`.

See `ps2/README.txt` for instructions for downloading and installing LIBLINEAR. Similar to part (c), train an SVM with training set sizes 50, 100, 200, . . . , 1400, by using the file `MATRIX.TRAIN.50` and so on. Plot the test error each time, using `MATRIX.TEST` as the test data. Use the LIBLINEAR default options when training and testing. You don't need to try different parameter values.

Running LIBLINEAR in Matlab on Windows or Octave can be buggy, depending on which version of Windows you run. We recommend that you use Matlab on the corn machines (e.g., ssh to corn.stanford.edu). However, there are command line programs you can run (without using MATLAB) which are located in `liblinear-1.7/windows` for Windows and `liblinear-1.7/` for Linux/Unix. If you do it this way, please include the commands that you run from the command line in your solution.

(e) How do naive Bayes and Support Vector Machines compare (in terms of generalization error) as a function of the training set size?

4. **[20 points] Properties of VC dimension**

In this problem, we investigate a few properties of the Vapnik-Chervonenkis dimension, mostly relating to how VC(H) increases as the set H increases. For each part of this problem, you should state whether the given statement is true, and justify your answer with either a formal proof or a counter-example.

(a) Let two hypothesis classes H_1 and H_2 satisfy $H_1 \subseteq H_2$. Prove or disprove: $\mathrm{VC}(H_1) \leq \mathrm{VC}(H_2)$.

(b) Let $H_1 = H_2 \cup \{h_1, \ldots, h_k\}$. (I.e., H_1 is the union of H_2 and some set of k additional hypotheses.) Prove or disprove: $\mathrm{VC}(H_1) \leq \mathrm{VC}(H_2) + k$. [Hint: You might want to start by considering the case of $k = 1$.]

(c) Let $H_1 = H_2 \cup H_3$. Prove or disprove: $\mathrm{VC}(H_1) \leq \mathrm{VC}(H_2) + \mathrm{VC}(H_3)$.

5. **[20 points] Training and testing on different distributions**

In the discussion in class about learning theory, a key assumption was that we trained and tested our learning algorithms on the same distribution $\mathcal{D}$. In this problem, we'll investigate one special case of training and testing on different distributions. Specifically, we will consider what happens when the training labels are *noisy*, but the test labels are not.

Consider a binary classification problem with labels $y \in \{0, 1\}$, and let $\mathcal{D}$ be a distribution over (x, y), that we'll think of as the original, "clean" or "uncorrupted" distribution. Define $\mathcal{D}_\tau$ to be a "corrupted" distribution over (x, y) which is the same as $\mathcal{D}$, except that the labels y have some probability $0 \leq \tau < 0.5$ of being flipped. Thus, to sample from $\mathcal{D}_\tau$, we would first sample (x, y) from $\mathcal{D}$, and then with probability τ (independently of the observed x and y) replace y with $1 - y$. Note that $\mathcal{D}_0 = \mathcal{D}$.

The distribution $\mathcal{D}_\tau$ models a setting in which an unreliable human (or other source) is labeling your training data for you, and on each example he/she has a probability τ of mislabeling it. Even though our training data is corrupted, we are still interested in evaluating our hypotheses with respect to the original, uncorrupted distribution $\mathcal{D}$.

We define the generalization error *with respect to* $\mathcal{D}_\tau$ to be

$$\varepsilon_\tau(h) = P_{(x,y)\sim\mathcal{D}_\tau}[h(x) \neq y].$$

Note that $\varepsilon_0(h)$ is the generalization error with respect to the "clean" distribution; it is with respect to ε_0 that we wish to evaluate our hypotheses.

(a) For any hypothesis h, the quantity $\varepsilon_0(h)$ can be calculated as a function of $\varepsilon_\tau(h)$ and τ. Write down a formula for $\varepsilon_0(h)$ in terms of $\varepsilon_\tau(h)$ and τ, and justify your answer.

(b) Let $|H|$ be finite, and suppose our training set $S = \{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$ is obtained by drawing m examples IID from the corrupted distribution $\mathcal{D}_\tau$. Suppose we pick $h \in H$ using empirical risk minimization: $\hat{h} = \arg\min_{h\in H} \hat{\varepsilon}_S(h)$. Also, let $h^* = \arg\min_{h\in H} \varepsilon_0(h)$.

Let any $\delta, \gamma > 0$ be given. Prove that for

$$\varepsilon_0(\hat{h}) \leq \varepsilon_0(h^*) + 2\gamma$$

to hold with probability $1 - \delta$, it suffices that

$$m \geq \frac{1}{2(1-2\tau)^2\gamma^2} \log \frac{2|H|}{\delta}.$$

Remark. This result suggests that, roughly, m examples that have been corrupted at noise level τ are worth about as much as $(1 - 2\tau)^2 m$ uncorrupted training examples. This is a useful rule-of-thumb to know if you ever need to decide whether/how much to pay for a more reliable source of training data. (If you've taken a class in information theory, you may also have heard that $(1-\mathcal{H}(\tau))m$ is a good estimate of the information in the m corrupted examples, where $\mathcal{H}(\tau) = -(\tau \log_2 \tau + (1-\tau)\log_2(1-\tau))$ is the "binary entropy" function. And indeed, the functions $(1-2\tau)^2$ and $1-\mathcal{H}(\tau)$ are quite close to each other.)

(c) Comment **briefly** on what happens as τ approaches 0.5.

CS229: Machine Learning

Problem Set #: ____

Please print out, fill in and include this cover sheet as the first page of your submission. We strongly recommend that you use this cover sheet, which will help us to get your graded homework back to you more quickly, as well as help us with tracking submissions.

Please mark the submission time clearly below. It is an honor code violation to write down the wrong time.

If you are submitting this homework late: Each student will have a total of **seven free late (calendar) days** to use for homeworks, project proposals and project milestones. Once these late days are exhausted, any assignments turned in late will be penalized 20% per late day. However, no assignment will be accepted **more than four days** after its due date, and late days cannot be used for the final project writeup. Each 24 hours or part thereof that a homework is late uses up one full late day.

On-campus (non-SCPD) students: Please either hand in the assignment at the beginning of class on Wednesday or leave it in the submission cabinet on the 1st floor of the Gates building, near/outside Gates 188 and 182.

Name: ____

SUNet ID: ______________________________@stanford.edu

Submission date: ________________ and time: ___________

Collaborators: ____________________________________

I understand and acknowledge CS229's Honor Code Policy (available online at http://cs229.stanford.edu/info.html)

Signature: ______________________________________

(For CS229 staff only)

Question	Score
1	
2	
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5	
6	
Late Days	
Total	

CS 229, Autumn 2013 Problem Set #2 Solutions: Naive Bayes, SVMs, and Theory

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1. **[15 points] Constructing kernels**

   In class, we saw that by choosing a kernel $K(x,z) = \phi(x)^T\phi(z)$, we can implicitly map data to a high dimensional space, and have the SVM algorithm work in that space. One way to generate kernels is to explicitly define the mapping ϕ to a higher dimensional space, and then work out the corresponding K.

   However in this question we are interested in direct construction of kernels. I.e., suppose we have a function $K(x,z)$ that we think gives an appropriate similarity measure for our learning problem, and we are considering plugging K into the SVM as the kernel function. However for $K(x,z)$ to be a valid kernel, it must correspond to an inner product in some higher dimensional space resulting from some feature mapping ϕ. Mercer's theorem tells us that $K(x,z)$ is a (Mercer) kernel if and only if for any finite set $\{x^{(1)},\ldots,x^{(m)}\}$, the matrix K is symmetric and positive semidefinite, where the square matrix $K \in \mathbb{R}^{m\times m}$ is given by $K_{ij} = K(x^{(i)}, x^{(j)})$.

   Now here comes the question: Let K_1, K_2 be kernels over $\mathbb{R}^n \times \mathbb{R}^n$, let $a \in \mathbb{R}^+$ be a positive real number, let $f : \mathbb{R}^n \mapsto \mathbb{R}$ be a real-valued function, let $\phi : \mathbb{R}^n \to \mathbb{R}^d$ be a function mapping from $\mathbb{R}^n$ to $\mathbb{R}^d$, let K_3 be a kernel over $\mathbb{R}^d \times \mathbb{R}^d$, and let $p(x)$ a polynomial over x with *positive* coefficients.

   For each of the functions K below, state whether it is necessarily a kernel. If you think it is, prove it; if you think it isn't, give a counter-example.

   (a) $K(x,z) = K_1(x,z) + K_2(x,z)$

   (b) $K(x,z) = K_1(x,z) - K_2(x,z)$

(c) $K(x,z) = aK_1(x,z)$

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(e) $K(x,z) = K_1(x,z)K_2(x,z)$

(f) $K(x,z) = f(x)f(z)$

(g) $K(x,z) = K_3(\phi(x), \phi(z))$

(h) $K(x,z) = p(K_1(x,z))$

[Hint: For part (e), the answer is that the K there *is* indeed a kernel. You still have to prove it, though. (This one may be harder than the rest.) This result may also be useful for another part of the problem.]

Answer: All 8 cases of proposed kernels K are trivially symmetric because K_1, K_2, K_3 are symmetric; and because the product of 2 real numbers is commutative (for (1f)). Thanks to Mercer's theorem, it is sufficient to prove the corresponding properties for positive semidefinite matrices. To differentiate between matrix and kernel function, we'll use G_i to denote a kernel matrix (Gram matrix) corresponding to a kernel function K_i.

(a) Kernel. The sum of 2 positive semidefinite matrices is a positive semidefinite matrix: $\forall z\ z^T G_1 z \geq 0, z^T G_2 z \geq 0$ since K_1, K_2 are kernels. This implies $\forall z\ z^T G z = z^T G_1 z + z^T G_2 z \geq 0$.

(b) Not a kernel. Counterexample: let $K_2 = 2K_1$ (we are using (1c) here to claim K_2 is a kernel). Then we have $\forall z\ z^T G z = z^T(G_1 - 2G_1)z = -z^T G_1 z \leq 0$.

(c) Kernel. $\forall z\ z^T G_1 z \geq 0$, which implies $\forall z\ a z^T G_1 z \geq 0$.

(d) Not a kernel. Counterexample: $a = 1$. Then we have $\forall z\ -z^T G_1 z \leq 0$.

(e) Kernel. K_1 is a kernel, thus $\exists \phi^{(1)}\ K_1(x,z) = \phi^{(1)}(x)^T \phi^{(1)}(z) = \sum_i \phi_i^{(1)}(x)\phi_i^{(1)}(z)$. Similarly, K_2 is a kernel, thus $\exists \phi^{(2)}\ K_2(x,z) = \phi^{(2)}(x)^T \phi^{(2)}(z) = \sum_j \phi_j^{(2)}(x)\phi_j^{(2)}(z)$.

$$\begin{aligned}
K(x,z) &= K_1(x,z)K_2(x,z) && (1)\\
&= \sum_i \phi_i^{(1)}(x)\phi_i^{(1)}(z) \sum_i \phi_i^{(2)}(x)\phi_i^{(2)}(z) && (2)\\
&= \sum_i \sum_j \phi_i^{(1)}(x)\phi_i^{(1)}(z)\phi_j^{(2)}(x)\phi_j^{(2)}(z) && (3)\\
&= \sum_i \sum_j (\phi_i^{(1)}(x)\phi_j^{(2)}(x))(\phi_i^{(1)}(z)\phi_j^{(2)}(z)) && (4)\\
&= \sum_{(i,j)} \psi_{i,j}(x)\psi_{i,j}(z) && (5)
\end{aligned}$$

Where the last equality holds because that's how we define ψ. We see K can be written in the form $K(x,z) = \psi(x)^T\psi(z)$ so it is a kernel.

(f) Kernel. Just let $\psi(x) = f(x)$, and since $f(x)$ is a scalar, we have $K(x,z) = \phi(x)^T\phi(z)$ and we are done.

(g) Kernel. Since K_3 is a kernel, the matrix G_3 obtained for *any* finite set $\{x^{(1)}, \ldots, x^{(m)}\}$ is positive semidefinite, and so it is also positive semidefinite for the sets $\{\phi(x^{(1)}), \ldots, \phi(x^{(m)})\}$.

(h) Kernel. By combining (1a) sum, (1c) scalar product, (1e) powers, (1f) constant term, we see that any polynomial of a kernel K_1 will again be a kernel.

2. **[15 points] Kernelizing the Perceptron**

   Let there be a binary classification problem with $y \in \{0, 1\}$. The perceptron uses hypotheses of the form $h_\theta(x) = g(\theta^T x)$, where $g(z) = \mathbf{1}\{z \geq 0\}$. In this problem we will consider a stochastic gradient descent-like implementation of the perceptron algorithm where each update to the parameters θ is made using only one training example. However, unlike stochastic gradient descent, the perceptron algorithm will only make one pass through the entire training set. The update rule for this version of the perceptron algorithm is given by

$$\theta^{(i+1)} := \theta^{(i)} + \alpha[y^{(i+1)} - h_{\theta^{(i)}}(x^{(i+1)})]x^{(i+1)}$$

   where $\theta^{(i)}$ is the value of the parameters after the algorithm has seen the first i training examples. Prior to seeing any training examples, $\theta^{(0)}$ is initialized to $\vec{0}$.

   Let K be a Mercer kernel corresponding to some very high-dimensional feature mapping ϕ. Suppose ϕ is so high-dimensional (say, ∞-dimensional) that it's infeasible to ever represent $\phi(x)$ explicitly. Describe how you would apply the "kernel trick" to the perceptron to make it work in the high-dimensional feature space ϕ, but without ever explicitly computing $\phi(x)$. [Note: You don't have to worry about the intercept term. If you like, think of ϕ as having the property that $\phi_0(x) = 1$ so that this is taken care of.] Your description should specify

   (a) How you will (implicitly) represent the high-dimensional parameter vector $\theta^{(i)}$, including how the initial value $\theta^{(0)} = \vec{0}$ is represented (note that $\theta^{(i)}$ is now a vector whose dimension is the same as the feature vectors $\phi(x)$);

   (b) How you will efficiently make a prediction on a new input $x^{(i+1)}$. I.e., how you will compute $h_{\theta^{(i)}}(x^{(i+1)}) = g({\theta^{(i)}}^T \phi(x^{(i+1)}))$, using your representation of $\theta^{(i)}$; and

   (c) How you will modify the update rule given above to perform an update to θ on a new training example $(x^{(i+1)}, y^{(i+1)})$; i.e., using the update rule corresponding to the feature mapping ϕ:

$$\theta^{(i+1)} := \theta^{(i)} + \alpha[y^{(i+1)} - h_{\theta^{(i)}}(\phi(x^{(i+1)}))]\phi(x^{(i+1)})$$

   [Note: If you prefer, you are also welcome to do this problem using the convention of labels $y \in \{-1, 1\}$, and $g(z) = \text{sign}(z) = 1$ if $z \geq 0$, -1 otherwise.]

   Answer:

   In the high-dimensional space we update θ as follows:

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

   So (assuming we initialize $\theta^{(0)} = \vec{0}$) θ will always be a linear combination of the $\phi(x^{(i)})$, i.e., $\exists \beta_l$ such that $\theta^{(i)} = \sum_{l=1}^{i} \beta_l \phi(x^{(l)})$ after having incorporated i training points. Thus $\theta^{(i)}$ can be compactly represented by the coefficients β_l of this linear combination, i.e., i real numbers after having incorporated i training points $x^{(i)}$. The initial value $\theta^{(0)}$ simply corresponds to the case where the summation has no terms (i.e., an empty list of coefficients β_l).

   We do not work explicitly in the high-dimensional space, but use the fact that $g({\theta^{(i)}}^T \phi(x^{(i+1)})) = g(\sum_{l=1}^{i} \beta_l \cdot \phi(x^{(l)})^T \phi(x^{i+1})) = g(\sum_{l=1}^{i} \beta_l K(x^{(l)}, x^{(i+1)}))$, which can be computed efficiently.

   We can efficiently update θ. We just need to compute $\beta_i = \alpha(y^{(i)} - g({\theta^{(i-1)}}^T \phi(x^{(i)})))$ at iteration i. This can be computed efficiently, if we compute ${\theta^{(i-1)}}^T \phi(x^{(i)})$ efficiently as described above.

In an alternative approach, one can observe that, unless a sample $\phi(x^{(i)})$ is misclassified, $y^{(i)} - h_{\theta^{(i)}}(\phi(x^{(i)}))$ will be zero; otherwise, it will be ± 1 (or ± 2, if the convention $y, h \in \{-1, 1\}$ is taken). The vector θ, then, can be represented as the sum $\sum_{\{i: y^{(i)} \neq h_{\theta^{(i)}}(\phi(x^{(i)}))\}} \alpha(2y^{(i)} - 1)\phi(x^{(i)})$ under the $y, h \in \{0, 1\}$ convention, and containing $(2y^{(i)})$ under the other convention. This can then be expressed as $\theta^{(i)} = \sum_{i \in \text{Misclassified}} \beta_i \phi(x^{(i)})$ to be in more obvious congruence with the above. The efficient representation can now be said to be a list which stores only those indices that were misclassified, as the β_is can be recomputed from the $y^{(i)}$s and α on demand. The derivation for (b) is then only cosmetically different, and in (c) the update rule is to add $(i + 1)$ to the list if $\phi(x^{(i+1)})$ is misclassified.

3. **[30 points] Spam classification**

   In this problem, we will use the naive Bayes algorithm and an SVM to build a spam classifier.

   In recent years, spam on electronic newsgroups has been an increasing problem. Here, we'll build a classifier to distinguish between "real" newsgroup messages, and spam messages. For this experiment, we obtained a set of spam emails, and a set of genuine newsgroup messages.[1] Using only the subject line and body of each message, we'll learn to distinguish between the spam and non-spam.

   All the files for the problem are in `/afs/ir/class/cs229/ps/ps2/`. **Note: Please do not circulate this data outside this class.** In order to get the text emails into a form usable by naive Bayes, we've already done some preprocessing on the messages. You can look at two sample spam emails in the files `spam_sample_original*`, and their preprocessed forms in the files `spam_sample_preprocessed*`. The first line in the preprocessed format is just the label and is not part of the message. The preprocessing ensures that only the message body and subject remain in the dataset; email addresses (EMAILADDR), web addresses (HTTPADDR), currency (DOLLAR) and numbers (NUMBER) were also replaced by the special tokens to allow them to be considered properly in the classification process. (In this problem, we'll going to call the features "tokens" rather than "words," since some of the features will correspond to special values like EMAILADDR. You don't have to worry about the distinction.) The files `news_sample_original` and `news_sample_preprocessed` also give an example of a non-spam mail.

   The work to extract feature vectors out of the documents has also been done for you, so you can just load in the design matrices (called document-word matrices in text classification) containing all the data. In a document-word matrix, the i^{th} row represents the i^{th} document/email, and the j^{th} column represents the j^{th} distinct token. Thus, the (i, j)-entry of this matrix represents the number of occurrences of the j^{th} token in the i^{th} document.

   For this problem, we've chosen as our set of tokens considered (that is, as our vocabulary) only the medium frequency tokens. The intuition is that tokens that occur too often or too rarely do not have much classification value. (Examples tokens that occur very often are words like "the," "and," and "of," which occur in so many emails and are sufficiently content-free that they aren't worth modeling.) Also, words were stemmed using a standard stemming algorithm; basically, this means that "price," "prices" and "priced" have all been replaced with "price," so that they can be treated as the same word. For a list of the tokens used, see the file `TOKENS_LIST`.

[1] Thanks to Christian Shelton for providing the spam email. The non-spam messages are from the 20 newsgroups data at http://www-2.cs.cmu.edu/afs/cs.cmu.edu/project/theo-20/www/data/news20.html .

Since the document-word matrix is extremely sparse (has lots of zero entries), we have stored it in our own efficient format to save space. You don't have to worry about this format.[2] The file `readMatrix.m` provides the `readMatrix` function that reads in the document-word matrix and the correct class labels for the various documents. Code in `nb_train.m` and `nb_test.m` shows how `readMatrix` should be called. The documentation at the top of these two files will tell you all you need to know about the setup.

(a) Implement a naive Bayes classifier for spam classification, using the multinomial event model and Laplace smoothing.

You should use the code outline provided in `nb_train.m` to train your parameters, and then use these parameters to classify the test set data by filling in the code in `nb_test.m`. You may assume that any parameters computed in `nb_train.m` are in memory when `nb_test.m` is executed, and do not need to be recomputed (i.e., that `nb_test.m` is executed immediately after `nb_train.m`) [3].

Train your parameters using the document-word matrix in `MATRIX.TRAIN`, and then report the test set error on `MATRIX.TEST`.

Remark. If you implement naive Bayes the straightforward way, you'll find that the computed $p(x|y) = \prod_i p(x_i|y)$ often equals zero. This is because $p(x|y)$, which is the product of many numbers less than one, is a very small number. The standard computer representation of real numbers cannot handle numbers that are too small, and instead rounds them off to zero. (This is called "underflow.") You'll have to find a way to compute naive Bayes' predicted class labels without explicitly representing very small numbers such as $p(x|y)$. [Hint: Think about using logarithms.]

(b) Intuitively, some tokens may be particularly indicative of an email being in a particular class. We can try to get an informal sense of how indicative token i is for the SPAM class by looking at:

$$\log \frac{p(x_j = i|y = 1)}{p(x_j = i|y = 0)} = \log \left(\frac{P(\text{token } i|\text{email is SPAM})}{P(\text{token } i|\text{email is NOTSPAM})} \right).$$

Using the parameters fit in part (a), find the 5 tokens that are most indicative of the SPAM class (i.e., have the highest positive value on the measure above). The numbered list of tokens in the file `TOKENS_LIST` should be useful for identifying the words/tokens.

(c) Repeat part (a), but with training sets of size ranging from 50, 100, 200, ..., up to 1400, by using the files `MATRIX.TRAIN.*`. Plot the test error each time (use `MATRIX.TEST` as the test data) to obtain a learning curve (test set error vs. training set size). You may need to change the call to `readMatrix` in `nb_train.m` to read the correct file each time. Which training-set size gives the best test set error?

(d) Train an SVM on this dataset using the LIBLINEAR SVM library, available for download from http://www.csie.ntu.edu.tw/~cjlin/liblinear/. This implements an SVM using a linear kernel. Like the Naive Bayes implementation, an outline for your code is provided in `svm_train.m` and `svm_test.m`.

See `ps2/README.txt` for instructions for downloading and installing LIBLINEAR. Similar to part (c), train an SVM with training set sizes 50, 100, 200, ..., 1400,

[2] Unless you're not using Matlab/Octave, in which case feel free to ask us about it.

[3] Matlab note: If a .m file doesn't begin with a function declaration, the file is a script. Variables in a script are put into the global namespace, unlike with functions.

by using the file `MATRIX.TRAIN.50` and so on. Plot the test error each time, using `MATRIX.TEST` as the test data. Use the LIBLINEAR default options when training and testing. You don't need to try different parameter values.

Running LIBLINEAR in Matlab on Windows or Octave can be buggy, depending on which version of Windows you run. We recommend that you use Matlab on the corn machines (e.g., ssh to corn.stanford.edu). However, there are command line programs you can run (without using MATLAB) which are located in `liblinear-1.7/windows` for Windows and `liblinear-1.7/` for Linux/Unix. If you do it this way, please include the commands that you run from the command line in your solution.

(e) How do naive Bayes and Support Vector Machines compare (in terms of generalization error) as a function of the training set size?

Answer:

(a) The test error when training on the full training set was 1.63%. If you got a different error (or if you got the words `website` and `lowest` for part b), you most probably implemented the wrong Naive Bayes model.

(b) The five most indicative words for the spam class were: `httpaddr`, `spam`, `unsubscrib`, `ebai` and `valet`.

(c) The test set error for different training set set sizes was:

  i. Training set size 50: Test set error = 3.87%
  ii. Training set size 100: Test set error = 2.62%
  iii. Training set size 200: Test set error = 2.62%
  iv. Training set size 400: Test set error = 1.87%
  v. Training set size 800: Test set error = 1.75%
  vi. Training set size 1400: Test set error = 1.63%
  vii. Full training set: Test set error = 1.63%

(d) The test set error from the SVM for different training set sizes was:

  i. Training set size 50: Test set error = 5.25%
  ii. Training set size 100: Test set error = 3.12%
  iii. Training set size 200: Test set error = 1.25%
  iv. Training set size 400: Test set error = 1.50%
  v. Training set size 800: Test set error = 1.25%
  vi. Training set size 1400: Test set error = 1.00%
  vii. Full training set: Test set error = 0.63%

(e) The deduction that can be drawn is that Naive Bayes learns quickly with less data, but has higher asymptotic error. On the other hand, the SVM classifier has relatively higher error on very small training sets, but is asymptotically much better than Naive Bayes. Note that this is consistent with the observation discussed in class that generative learning algorithms (such as Naive Bayes) have smaller sample complexity than discriminative algorithms (such as SVMs), but may also have higher asymptotic error.

The Matlab code for the problem:

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% nb_train.m
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

[spmatrix, tokenlist, trainCategory] = readMatrix('MATRIX.TRAIN');

trainMatrix = full(spmatrix);
numTrainDocs = size(trainMatrix, 1);
numTokens = size(trainMatrix, 2);

% ...
% YOUR CODE HERE

V = size(trainMatrix, 2);
neg = trainMatrix(find(trainCategory == 0), :);
pos = trainMatrix(find(trainCategory == 1), :);

neg_words = sum(sum(neg));
pos_words = sum(sum(pos));

neg_log_prior = log(size(neg,1) / numTrainDocs);
pos_log_prior = log(size(pos,1) / numTrainDocs);

for k=1:V,
  neg_log_phi(k) = log((sum(neg(:,k)) + 1) / (neg_words + V));
  pos_log_phi(k) = log((sum(pos(:,k)) + 1) / (pos_words + V));
end


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% nb_test.m
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

[spmatrix, tokenlist, category] = readMatrix('MATRIX.TEST');

testMatrix = full(spmatrix);
numTestDocs = size(testMatrix, 1);
numTokens = size(testMatrix, 2);

% ...
output = zeros(numTestDocs, 1);

%---------------
% YOUR CODE HERE

for k=1:numTestDocs,
  [i,j,v] = find(testMatrix(k,:));
  neg_posterior = sum(v .* neg_log_phi(j)) + neg_log_prior;
```

```
    pos_posterior = sum(v .* pos_log_phi(j)) + pos_log_prior;

    if (neg_posterior > pos_posterior)
      output(k) = 0;
    else
      output(k) = 1;
    end
  end

  %---------------

  % Compute the error on the test set
  error=0;
  for i=1:numTestDocs
    if (category(i) ~= output(i))
      error=error+1;
    end
  end

  %Print out the classification error on the test set
  error/numTestDocs




  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  % svm_train.m
  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  % YOUR CODE HERE
  svm_category = 2.*trainCategory - 1;
  model = train(svm_category', sparseTrainMatrix)


  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  % svm_test.m
  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  % YOUR CODE HERE
  svm_category = 2.*testCategory - 1;
  [output, a] = predict(svm_category', sparseTestMatrix, model);
  output = 0.5.*(output + 1);
```

4. **[20 points] Properties of VC dimension**

   In this problem, we investigate a few properties of the Vapnik-Chervonenkis dimension, mostly relating to how VC(H) increases as the set H increases. For each part of this problem, you should state whether the given statement is true, and justify your answer with either a formal proof or a counter-example.

   (a) Let two hypothesis classes H_1 and H_2 satisfy $H_1 \subseteq H_2$. Prove or disprove: VC(H_1) $\leq$ VC(H_2).

(b) Let $H_1 = H_2 \cup \{h_1, \ldots, h_k\}$. (I.e., H_1 is the union of H_2 and some set of k additional hypotheses.) Prove or disprove: $\text{VC}(H_1) \leq \text{VC}(H_2) + k$. [Hint: You might want to start by considering the case of $k = 1$.]

(c) Let $H_1 = H_2 \cup H_3$. Prove or disprove: $\text{VC}(H_1) \leq \text{VC}(H_2) + \text{VC}(H_3)$.

Answer:

(a) True. Suppose that $VC(H_1) = d$. Then there exists a set of d points that is shattered by H_1 (i.e., for each possible labeling of the d points, there exists a hypothesis $h \in H_1$ which realizes that labeling). Now, since H_2 contains all hypotheses in H_1, then H_2 shatters the same set, and thus we have $VC(H_2) \geq d = VC(H_1)$.

(b) True. If we can prove the result for $k = 1$, then the result stated in the problem set follows immediately by applying the same logic inductively, one hypothesis at a time. So, let us prove that if $H_1 = H_2 \cup \{h\}$, then $VC(H_1) \leq VC(H_2) + 1$. Suppose that $VC(H_1) = d$, and let S_1 be a set of d points that is shattered by H_1. Now, pick an arbitrary $x \in S_1$. Since H_1 shatters S_1, there must be some $\bar{h} \in H_1$ such that h and $\bar{h}$ agree on labelings for all points in S_1 except x. This means that $H' := H_1 \setminus \{h\}$ achieves all possible labelings on $S' := S_1 \setminus \{x\}$ (i.e. H' shatters S'), so $VC(H') \geq |S'| = d - 1$. But $H' \subseteq H_2$, so from part (a), $VC(H') \leq VC(H_2)$. It follows that $VC(H_2) \geq d - 1$, or equivalently, $VC(H_1) \leq VC(H_2) + 1$, as desired.

For this problem, there were a number of possible correct proof methods; generally, to get full credit, you needed to argue formally that there exists no set of $(VC(H_2) + 2)$ points shattered by H_1, or equivalently, that there always exists a set of $(VC(H_1) - 1)$ points shattered by H_2. Here are a couple of the more common errors:

- Some submitted solutions stated that adding a single hypothesis to H_2 increases the VC dimension by at most one, since the new hypothesis can only realize a single labeling. While this statement is vaguely true, it is neither sufficiently precise, nor is its correctness immediately obvious.
- Some solutions made arguments relating to the cardinality of the sets H_1 and H_2. However, generally when we speak about VC dimension, the sets H_1 and H_2 often have infinite cardinality (e.g., the set of all linear classifiers in $\mathbb{R}^2$).

(c) False. Counterexample: let $H_1 = \{h_1\}, H_2 = \{h_2\}$, and $\forall x,\ h_1(x) = 0, h_2(x) = 1$. Then we have $VC(H_1) = VC(H_2) = 0$, but $VC(H_1 \cup H_2) = 1$.

5. **[20 points] Training and testing on different distributions**

In the discussion in class about learning theory, a key assumption was that we trained and tested our learning algorithms on the same distribution $\mathcal{D}$. In this problem, we'll investigate one special case of training and testing on different distributions. Specifically, we will consider what happens when the training labels are *noisy*, but the test labels are not.

Consider a binary classification problem with labels $y \in \{0, 1\}$, and let $\mathcal{D}$ be a distribution over (x, y), that we'll think of as the original, "clean" or "uncorrupted" distribution. Define $\mathcal{D}_\tau$ to be a "corrupted" distribution over (x, y) which is the same as $\mathcal{D}$, except that the labels y have some probability $0 \leq \tau < 0.5$ of being flipped. Thus, to sample from $\mathcal{D}_\tau$, we would first sample (x, y) from $\mathcal{D}$, and then with probability τ (independently of the observed x and y) replace y with $1 - y$. Note that $\mathcal{D}_0 = \mathcal{D}$.

The distribution $\mathcal{D}_\tau$ models a setting in which an unreliable human (or other source) is labeling your training data for you, and on each example he/she has a probability τ of mislabeling it. Even though our training data is corrupted, we are still interested in evaluating our hypotheses with respect to the original, uncorrupted distribution $\mathcal{D}$.

We define the generalization error *with respect to* $\mathcal{D}_\tau$ to be

$$\varepsilon_\tau(h) = P_{(x,y)\sim\mathcal{D}_\tau}[h(x) \neq y].$$

Note that $\varepsilon_0(h)$ is the generalization error with respect to the "clean" distribution; it is with respect to ε_0 that we wish to evaluate our hypotheses.

(a) For any hypothesis h, the quantity $\varepsilon_0(h)$ can be calculated as a function of $\varepsilon_\tau(h)$ and τ. Write down a formula for $\varepsilon_0(h)$ in terms of $\varepsilon_\tau(h)$ and τ, and justify your answer.

(b) Let $|H|$ be finite, and suppose our training set $S = \{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$ is obtained by drawing m examples IID from the corrupted distribution $\mathcal{D}_\tau$. Suppose we pick $h \in H$ using empirical risk minimization: $\hat{h} = \arg\min_{h\in H} \hat{\varepsilon}_S(h)$. Also, let $h^* = \arg\min_{h\in H} \varepsilon_0(h)$.

Let any $\delta, \gamma > 0$ be given. Prove that for

$$\varepsilon_0(\hat{h}) \leq \varepsilon_0(h^*) + 2\gamma$$

to hold with probability $1 - \delta$, it suffices that

$$m \geq \frac{1}{2(1-2\tau)^2\gamma^2} \log \frac{2|H|}{\delta}.$$

Remark. This result suggests that, roughly, m examples that have been corrupted at noise level τ are worth about as much as $(1-2\tau)^2 m$ uncorrupted training examples. This is a useful rule-of-thumb to know if you ever need to decide whether/how much to pay for a more reliable source of training data. (If you've taken a class in information theory, you may also have heard that $(1-\mathcal{H}(\tau))m$ is a good estimate of the information in the m corrupted examples, where $\mathcal{H}(\tau) = -(\tau \log_2 \tau + (1-\tau)\log_2(1-\tau))$ is the "binary entropy" function. And indeed, the functions $(1-2\tau)^2$ and $1-\mathcal{H}(\tau)$ are quite close to each other.)

(c) Comment **briefly** on what happens as τ approaches 0.5.

Answer:

(a) We compute ε_τ as a function of ε_0 and then invert the obtained expression. An error occurs on the corrupted distribution, if and only if, an error occurred for the original distribution and the point that was not corrupted, or no error occurred for the original distribution but the point was corrupted. So we have

$$\varepsilon_\tau = \varepsilon_0(1-\tau) + (1-\varepsilon_0)\tau$$

Solving for ε_0 gives

$$\varepsilon_0 = \frac{\varepsilon_\tau - \tau}{1-2\tau}$$

(b) We will need to apply the following (in the right order):

$$\forall h \in H,\ |\varepsilon_\tau(h) - \hat{\varepsilon}_\tau(h)| \le \bar{\gamma} \quad \text{w.p.}(1-\delta), \quad \delta = 2K\exp(-2\bar{\gamma}^2 m) \tag{6}$$

$$\varepsilon_\tau = (1-2\tau)\varepsilon + \tau, \quad \varepsilon_0 = \frac{\varepsilon_\tau - \tau}{1-2\tau} \tag{7}$$

$$\forall h \in H,\ \hat{\varepsilon}_\tau(\hat{h}) \le \hat{\varepsilon}_\tau(h), \quad \text{in particular for } h^* \tag{8}$$

Here is the derivation:

$$\begin{aligned}
\varepsilon_0(\hat{h}) &= \frac{\varepsilon_\tau(\hat{h}) - \tau}{1-2\tau} && (9)\\
&\le \frac{\hat{\varepsilon}_\tau(\hat{h}) + \bar{\gamma} - \tau}{1-2\tau} \quad \text{w.p.}(1-\delta) && (10)\\
&\le \frac{\hat{\varepsilon}_\tau(h^*) + \bar{\gamma} - \tau}{1-2\tau} \quad \text{w.p.}(1-\delta) && (11)\\
&\le \frac{\varepsilon_\tau(h^*) + 2\bar{\gamma} - \tau}{1-2\tau} \quad \text{w.p.}(1-\delta) && (12)\\
&= \frac{(1-2\tau)\varepsilon_0(h^*) + \tau + 2\bar{\gamma} - \tau}{1-2\tau} \quad \text{w.p.}(1-\delta) && (13)\\
&= \varepsilon_0(h^*) + \frac{2\bar{\gamma}}{1-2\tau} \quad \text{w.p.}(1-\delta) && (14)\\
&= \varepsilon_0(h^*) + 2\gamma \quad \text{w.p.}(1-\delta) && (15)
\end{aligned}$$

Where we used in the following order: (7)(6)(8)(6)(7), and the last 2 steps are algebraic simplifications, and defining γ as a function of $\bar{\gamma}$. Now we can fill out $\bar{\gamma} = \gamma(1-2\tau)$ into δ of (6), solve for m and we are done.

Note: one could shorten the above derivation and go straight from (9) to (12) by using that result from class.

(c) The closer τ is to 0.5, the more samples are needed to get the same generalization error bound. For τ approaching 0.5, the training data becomes more and more random; having no information at all about the underlying distribution for $\tau = 0.5$.