In [1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.datasets import load_iris
from sklearn.metrics import classification_report

%matplotlib inline
```

本文主要参考了以下材料：
1. cs229: *9.3 softmax regression*
2. http://ufldl.stanford.edu/wiki/index.php/Softmax%E5%9B%9E%E5%BD%92 (http://ufldl.stanford.edu/wiki/index.php/Softmax%E5%9B%9E%E5%BD%92)
3. https://blog.csdn.net/u012328159/article/details/72155874 (https://blog.csdn.net/u012328159/article/details/72155874)

Softmax Regression

1. 原理推导

Consider a classification problem in which the response variable y can take on any one of k values, so $y \in \{1, 2, \ldots, k\}$. The response variable is still discrete, but can now take on more than two values. We will thus model it as distributed according to a multinomial distribution.

Lets derive a GLM for modelling this type of multinomial data. To do so, we will begin by expressing the multinomial as an exponential family distribution.

To parameterize a multinomial over k possible outcomes, one could use k parameters $\phi_1, \ldots, \phi_k$ specifying the probability of each of the outcomes. However, these parameters would be redundant, or more formally, they would not be independent (since knowing any $k-1$ of the ϕ_i's uniquely determines the last one, as they must satisfy $\sum_{i=1}^{k}\phi_i = 1$). So, we will instead parameterize the multinomial with only $k-1$ parameters, $\phi_1, \dots, \phi_{k-1}$, where $\phi_i = p(y=i;\phi)$, and $p(y=k;\phi) = 1 - \sum_{i=1}^{k-1}\phi_i$. For notational convenience, we will also let $\phi_k = 1 - \sum_{i=1}^{k-1}\phi_i$, but we should keep in mind that this is not a parameter, and that it is fully specified by $\phi_1, \dots, \phi_{k-1}$.

To express the multinomial as an exponential family distribution, we will define $T(y) \in \mathbb{R}^{k-1}$ as follows:

$$T(1) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, T(2) = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, T(3) = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \cdots, T(k-1) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}, T(k) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

Unlike our previous examples, here we do not have $T(y) = y$; also, $T(y)$ is now a $k-1$ dimensional vector, rather than a real number. We will write $(T(y))_i$ to denote the i-th element of the vector $T(y)$.

We introduce one more very useful piece of notation. An indicator function $1\{\cdot\}$ takes on a value of 1 if its argument is true, and 0 otherwise. So, we can write the relationship between $T(y)$ and y as $(T(y))_i = 1\{y=i\}$ (当且仅当$y=i$时，向量$T(y)$的第i个位置元素为1). Further, we have that $E[(T(y))_i] = P(y=i) = \phi_i$.

We are now ready to show that the multinomial is a member of the exponential family. We have:

$$
\begin{aligned}
p(y;\phi) &= \phi_1^{1\{y=1\}} \phi_2^{1\{y=2\}} \cdots \phi_k^{1\{y=k\}} \\
&= \phi_1^{1\{y=1\}} \phi_2^{1\{y=1\}} \cdots \phi_k^{1-\sum_{i=1}^{k-1} 1\{y=i\}} \\
&= \phi_1^{(T(y))_1} \phi_2^{(T(y))_2} \cdots \phi_k^{1-\sum_{i=1}^{k-1}(T(y))_i} \\
&= exp((T(y))_1 log(\phi_1) + (T(y))_2 log(\phi_2) + \cdots + (1 - \sum_{i=1}^{k-1}(T(y))_i) log(\phi_k)) \\
&= exp((T(y))_1 log(\frac{\phi_1}{\phi_k}) + (T(y))_2 log(\frac{\phi_2}{\phi_k}) + \cdots + (T(y))_{k-1} log(\frac{\phi_{k-1}}{\phi_k}) + log(\phi_k)) \\
&= b(y)\, exp(\eta^T T(y) - a(\eta))
\end{aligned}
$$

where

$$
\eta = \begin{bmatrix} log(\frac{\phi_1}{\phi_k}) \\ log(\frac{\phi_2}{\phi_k}) \\ \vdots \\ log(\frac{\phi_{k-1}}{\phi_k}) \end{bmatrix}
$$

$$
a(\eta) = -log(\phi_k)
$$

$$
b(y) = 1
$$

This completes our formulation of the multinomial as an exponential family distribution.

The link function is given (for $i = 1, \cdots, k$) by

$$\eta_i = log\frac{\phi_i}{\phi_k}$$

For convenience, we have also defined $\eta_k = log(\frac{\phi_k}{\phi_k}) = 0$. To invert the link function and derive the response function, we therefore have that

$$e^{\eta_i} = \frac{\phi_i}{\phi_k}$$

$$\phi_k e^{\eta_i} = \phi_i \qquad -(1)$$

$$\phi_k \sum_{i=1}^{k} e^{\eta_i} = \sum_{i=1}^{k} \phi_i = 1$$

This implies that $\phi_k = 1/\sum_{i=1}^{k} e^{\eta_i}$, which can be substituted back into Equation (1) to give the response function

$$\phi_i = \frac{e^{\eta_i}}{\sum_{l=1}^{k} e^{\eta_l}}$$

This function mapping from the η's to the ϕ's is called the **softmax function**.

To complete our model, we use Assumption 3, given earlier, that the η's are linearly related to the x's. So, have $\eta_i = \theta_i^T x$ (for $i = 1, \cdots, k-1$), where $\theta_1, \cdots, \theta_{k-1} \in \mathbb{R}^{n+1}$ are the parameters of our model. For notational convenience, we can also define $\theta_k = 0$, so that $\eta_k = \theta_k^T x = 0$, as given previously. Hence, our model assumes that the conditional distribution of y given x is given by

$$
\begin{aligned}
p(y=i|x;\theta) &= \phi_i \\
&= \frac{e^{\eta_i}}{\sum_{l=1}^{k} e^{\eta_l}} \\
&= \frac{e^{\theta_i^T x}}{\sum_{l=1}^{k} e^{\theta_l^T x}} \qquad -(2)
\end{aligned}
$$

This model, which applies to classification problems where $y \in \{1, \cdots, k\}$, is called **softmax regression**. It is a generalization of logistic regression.

Our hypothesis will output

$$
\begin{aligned}
h_\theta(x) &= E[T(y) \mid x; \theta] \\
&= E\left[\left.\begin{array}{c} 1\{y=1\} \\ 1\{y=2\} \\ \cdots \\ 1\{y=k-1\} \end{array}\right| x; \theta\right] \\
&= \begin{bmatrix} \phi_1 \\ \phi_2 \\ \cdots \\ \phi_{k-1} \end{bmatrix} \\
&= \begin{bmatrix} \frac{exp(\theta_1^T x)}{\sum_{l=1}^k exp(\theta_l^T x)} \\ \frac{exp(\theta_2^T x)}{\sum_{l=1}^k exp(\theta_l^T x)} \\ \vdots \\ \frac{exp(\theta_{k-1}^T x)}{\sum_{l=1}^k exp(\theta_l^T x)} \end{bmatrix}
\end{aligned}
$$

In other words, our hypothesis will output the estimated probability that $p(y = i|x; \theta)$, for every value of $i = 1, \cdots, k$(Even though $h_\theta(x)$ as defined above is only $k-1$ dimensional, clearly $p(y = k|x; \theta)$ can be obtained as $1 - \sum_{i=1}^{k-1} \phi_i$.)

Lastly, lets discuss parameter fitting. Similar to our original derivation of ordinary least squares and logistic regression, if we have a training set of m examples $\{(x^{(i)}, y^{(i)}); i = 1, \cdots, m\}$ and would like to learn the parameter θ_i of this model, we would begin by writing down the log-likelihood:

$$
\begin{aligned}
l(\theta) &= \sum_{i=1}^{m} logp(y^{(i)}|x^{(i)};\theta) \\
&= \sum_{i=1}^{m} log \prod_{j=1}^{k} \left(\frac{e^{\theta_j^T x^{(i)}}}{\sum_{i=l}^{k} e^{\theta_l^T x^{(i)}}} \right)^{1\{y^{(i)}=j\}} \\
&= \sum_{i=1}^{m} \sum_{j=1}^{k} 1\{y^{(i)} = j\} log \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}
\end{aligned}
$$

To obtain the second line above, we used the definition for $p(y|x;\theta)$ given in Equation (2). We can now obtain the maximum likelihood estimate of the parameters by maximizing $l(\theta)$ in terms of θ, using a method such as gradient ascent or Newton's method.

2. 梯度下降法

2.1 Cost Function

首先，定义

$$
x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \vdots \\ x_{n+1}^{(i)} \end{bmatrix}_{(n+1)\times 1} \qquad X = \begin{bmatrix} -(x^{(1)})^T- \\ -(x^{(2)})^T- \\ \cdots \\ -(x^{(m)})^T- \end{bmatrix}_{m\times(n+1)} \qquad \theta = \begin{bmatrix} -\theta_1^T- \\ -\theta_2^T- \\ \cdots \\ -\theta_k^T- \end{bmatrix}_{k\times(n+1)}
$$

注意到，$x^{(i)} \in \mathbb{R}^{n+1}$，其中定义$x_0^{(i)} = 0$。然后，$\theta_1, \theta_2, \cdots, \theta_k \in \mathbb{R}^{n+1}$，在这里，我没有定义$\theta_k = 0$，因

此，存在过度参数化的问题。所以，在接下来的小节内会对这个问题进行解决。最后，$y \in \{1, 2, \cdots, k\}$。

因此，我们定义Cost Function为

$$J(\theta) = -\frac{1}{m}\left(\sum_{i=1}^{m}\sum_{j=1}^{k} 1\{y^{(i)} = j\} log \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x}}\right)$$

值得注意的是，上述公式是逻辑回归的cost function的推广，逻辑回归的cost function可以改为：

$$\begin{aligned} J(\theta) &= -\frac{1}{m}\left(\sum_{i=1}^{m}(1 - y^{(i)}) log(1 - h_\theta(x^{(i)})) + y^{(i)} log h_\theta(x^{(i)})\right) \\ &= -\frac{1}{m}\left(\sum_{i=1}^{m}\sum_{j=0}^{1} 1\{y^{(i)} = j\} log\, p(y^{(i)} = j \mid x^{(i)}; \theta)\right) \end{aligned}$$

2.2 Softmax Regression 模型参数化的特点

由于上一节，我们没有定义 $\theta_k = 0$，这使得softmax regression有一个“冗余”的参数集。虽然，定义 $\theta_k = 0$ 可以避免这个问题，但是这会使得在算法实现中没有那么简单清楚，而且，这个问题是可以得到解决的。接下来，我们对这个问题进行具体说明。

假设我们从参数向量 θ_j 中减去了向量 ψ，这时，每一个 θ_j 都变成了 $\theta_j - \psi$ $(j = 1, \cdots, k)$。此时假设函数变成了以下的式子：

$$
\begin{aligned}
p(y^{(i)} = j \mid x^{(i)}; \theta) &= \frac{e^{(\theta_j - \psi)^T x^{(i)}}}{\sum_{l=1}^{k} e^{(\theta_l - \psi)^T x^{(i)}}} \\
&= \frac{e^{\theta_j^T x^{(i)}} e^{-\psi^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}} e^{-\psi^T x^{(i)}}} \\
&= \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}
\end{aligned}
$$

换句话说，从 θ_j 中减去 ψ 完全不影响假设函数的预测结果。这表明前面的softmax regression模型中存在冗余的参数。更正式一点说，softmax regression模型被过度参数化了。对于任意一个用于拟合数据的假设函数，可以求出多组参数值，这些参数得到的是完全相同的假设函数 h_θ。

进一步而言，如果参数 $(\theta_1, \theta_2, \cdots, \theta_k)$ 是 cost function $J(\theta)$ 的极小值点，那么 $(\theta_1 - \psi, \theta_2 - \psi, \cdots, \theta_k - \psi)$同样也是它的极小值点，其中 ψ 可以为任意向量。因此，使得 $J(\theta)$ 最小化的解不是唯一的。（有趣的是，由于 $J(\theta)$仍然是一个凸函数，因此梯度下降不会遇到局部最优解的问题，但是 $Hessian$ 矩阵是奇异的/不可逆的，这会直接导致采用牛顿法优化就遇到数值计算的问题）

注意，当 $\phi = \theta_k$ 时，我们总是可以将 θ_k 替换为 $\theta_k - \psi = \vec{0}$（即替换为全零向量），并且这种替换不会影响假设函数。因此，我们可以去掉参数向量 θ_k （或者其他 θ_j 中的任意一个）而不影响假设函数的表达能力。实际上，与其优化全部的 $k \times (n+1)$ 个参数 $(\theta_1, \theta_2, \cdots, \theta_k)$ （其中，$\theta_j \in \mathbb{R}^{n+1}$），我们可以令 $\theta_k = \vec{0}$，只优化剩余的 $(k-1) \times (n+1)$ 个参数，这样算法依然能够正常工作。

在实际应用中，为了让算法实现更加简单清楚，往往保留所有参数 $(\theta_1, \theta_2, \cdots, \theta_k)$，而不任意地将某一参数设置为 $\vec{0}$。但此时，我们需要对 cost function 做一个改动：加入权重衰减项。权重衰减项可以解决 softmax regression 参数冗余所带来的数值问题。

2.3 权重衰减

我们通过添加一个权重衰减项 $\frac{\lambda}{2}\sum_{i=1}^{k}\sum_{j=0}^{n}\theta_{ij}^2$ 来修改 cost function，这个衰减项会惩罚过大的参数值，现在我们的 cost function 变为：

$$J(\theta) = -\frac{1}{m}\left(\sum_{i=1}^{m}\sum_{j=1}^{k}1\{y^{(i)}=j\}\,log\,\frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k}e^{\theta_l^T x^{(i)}}}\right)+\frac{\lambda}{2}\sum_{i=1}^{k}\sum_{j=0}^{n}\theta_{ij}^2$$

有了这个权重衰减项之后($\lambda > 0$)，Cost function 就变成了严格的凸函数，这样就可以保证得到唯一的解了。此时的 Hessian 矩阵变成可逆矩阵，并且因为 $J(\theta)$ 是凸函数，梯度下降法和L-BFGS等算法可以保证收敛到全局最优解。

为了使用优化算法，我们需要求得这个新函数的 $J(\theta)$ 的导数，如下：

$$\nabla_{\theta_j}J(\theta) = -\frac{1}{m}\left(x^{(i)}(1\{y^{(i)}=j\}-p(y^{(i)}\mid x^{(i)};\theta))\right)+\lambda\theta_j$$

注意，这里的 $\nabla_{\theta_j}J(\theta)\in\mathbb{R}^{n+1}$。通过最小化 $J(\theta)$，我们就能实现一个可用的 softmax regression 模型。

2.4 推导 $\frac{\partial J(\theta)}{\partial\theta_j}$

方法一：

$$
\begin{aligned}
\frac{\partial J(\theta)}{\partial \theta_j} &= -\frac{1}{m}\frac{\partial}{\partial \theta_j}\left[\sum_{i=1}^{m}\sum_{j=1}^{k} 1\{y^{(i)} = j\}\, log\, \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}\right] + \lambda\theta_j \\
&= -\frac{1}{m}\frac{\partial}{\partial \theta_j}\left[\sum_{i=1}^{m}\sum_{j=1}^{k} 1\{y^{(i)} = j\}\, (log\, e^{\theta_j^T x^{(i)}} - log\, \sum_{l=1}^{k} e^{\theta_l^T x^{(i)}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\frac{\partial}{\partial \theta_j}\left[\sum_{i=1}^{m}\sum_{j=1}^{k} 1\{y^{(i)} = j\}\, (\theta_j^T x^{(i)} - log\, \sum_{l=1}^{k} e^{\theta_l^T x^{(i)}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\frac{\partial}{\partial \theta_j}\left[\sum_{i=1}^{m} 1\{y^{(i)} = j\}\, (\sum_{j=1}^{k}\theta_j^T x^{(i)} - \sum_{j=1}^{k} log\, \sum_{l=1}^{k} e^{\theta_l^T x^{(i)}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m} 1\{y^{(i)} = j\}\, (x^{(i)} - \sum_{j=1}^{k} \frac{x^{(i)} e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m} x^{(i)}\, (1\{y^{(i)} = j\} - \sum_{j=1}^{k} 1\{y^{(i)} = j\} \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m} x^{(i)}\, (1\{y^{(i)} = j\} - \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m} x^{(i)}\, (1\{y^{(i)} = j\} - p(y^{(i)} \mid x^{(i)}; \theta))\right] + \lambda\theta_j
\end{aligned}
$$

方法二：

$$
\begin{aligned}
\frac{\partial J(\theta)}{\partial \theta_j} &= -\frac{1}{m}\left[\sum_{i=1}^{m} \frac{\partial}{\partial \theta_j}(1\{y^{(i)}=j\}\, log\, \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}} + \sum_{c\neq j}^{k} 1\{y^{(i)}=c\}\, log\, \frac{e^{\theta_c^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}})\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m}(1\{y^{(i)}=j\}(x^{(i)} - \frac{x^{(i)} e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}) + \sum_{c\neq j}^{k} 1\{y^{(i)}=c\}(-\frac{x^{(i)} e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}))\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m}(x^{(i)} 1\{y^{(i)}=j\}(1 - \frac{e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}) + \sum_{c\neq j}^{k} 1\{y^{(i)}=c\}(-\frac{x^{(i)} e^{\theta_j^T x^{(i)}}}{\sum_{l=1}^{k} e^{\theta_l^T x^{(i)}}}))\right] + \lambda\theta_j \\
&= \frac{1}{m}\left[\sum_{i=1}^{m} x^{(i)}(1\{y^{(i)}=j\} - 1\{y^{(i)}=j\}p(y^{(i)} \mid x^{(i)};\theta)) + \sum_{c\neq j}^{k} 1\{y^{(i)}=c\}(-p(y^{(i)} \mid x^{(i)};\theta))\right] + \lambda\theta_j \\
&= \frac{1}{m}\left[\sum_{i=1}^{m} x^{(i)}(1\{y^{(i)}=j\} - \sum_{j=1}^{k} 1\{y^{(i)}=j\}p(y^{(i)} \mid x^{(i)};\theta)\right] + \lambda\theta_j \\
&= -\frac{1}{m}\left[\sum_{i=1}^{m} x^{(i)}\,(1\{y^{(i)}=j\} - p(y^{(i)} \mid x^{(i)};\theta))\right] + \lambda\theta_j
\end{aligned}
$$

2.5 矩阵化

因为 $y \in \{1, 2, \cdots, k\}$，所以，对 y 进行独热编码。即 $y^{(i)} \in \mathbb{R}^k$，其中，若 $y^{(i)}$ 属于类别 i，则 $y^{(i)}$ 第 i 个位置上的元素为1，其余位置元素为0。因此，定义矩阵 G 为

$$G = \begin{bmatrix} -(y^{(1)})^T- \\ -(y^{(2)})^T- \\ \vdots \\ -(y^{(m)})^T- \end{bmatrix}_{m\times k}$$

定义概率矩阵 P 为

$$P_{m\times k} = norm(\ exp(X_{m\times(n+1)} \cdot \theta^T_{(n+1)\times k})\ )$$

其中，norm 表示归一化项，因此，概率矩阵 P 的具体计算方式为：首先，计算 $exp(X\theta^T)$ 得到 $m \times k$ 的矩阵。其次，使用 $np.sum()$ 对该该矩阵按行进行求和，得到 m×1 的矩阵。最后，利用Python的广播（broadcast）机制，将该矩阵与 $exp(X\theta^T)$ 对应位置元素进行相乘（element-wise multiplication）得到概率矩阵 P。

于是

$$\frac{\partial J(\theta)}{\partial \theta} = -\frac{1}{m}(G-P)^T \cdot X + \lambda\theta$$

所以，cost function为

$$J(\theta) = -np.mean(G \circ P) + \lambda\ np.sum(\theta)$$

其中，$\circ$ 表示对应位置元素相乘，即 element-wise multiplication。

3. 实现 softmax regression

3.1 读取数据

In [2]:
```
iris = load_iris()
features = pd.DataFrame(data=iris.data, columns=iris.feature_names)
label = pd.DataFrame(data=iris.target, columns=['traget'])
data = pd.concat([features, label], axis=1)
data.head()
```

Out[2]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	traget
0	5.1	3.5	1.4	0.2	0
1	4.9	3.0	1.4	0.2	0
2	4.7	3.2	1.3	0.2	0
3	4.6	3.1	1.5	0.2	0
4	5.0	3.6	1.4	0.2	0

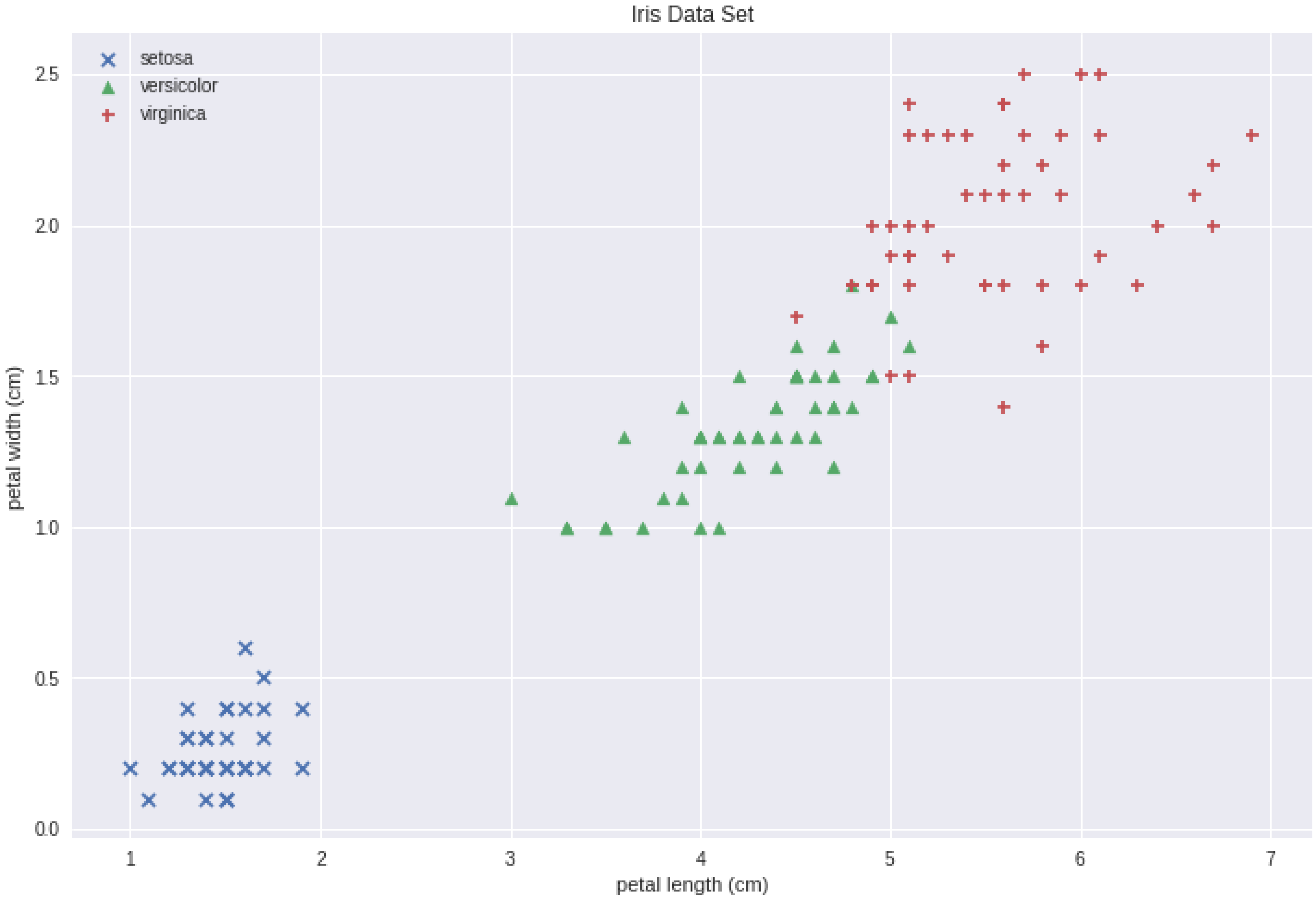
In [3]:
```
def loadData(df):
    ones = pd.DataFrame({'ones': np.ones(len(df))})
    df = pd.concat([ones, df], axis=1)
    X = df.iloc[:,:-1].values
    y = df.iloc[:,-1].values
    return X, y
```

In [4]:
```
X, y = loadData(data)
X.shape, y.shape
```

Out[4]: ((150, 5), (150,))

3.2 数据可视化

In [5]:
```
plt.figure(figsize=(12, 8))
plt.scatter(X[:, 3][y==0], X[:, 4][y==0], marker='x', label=iris.target_names[0])
plt.scatter(X[:, 3][y==1], X[:, 4][y==1], marker='^', label=iris.target_names[1])
plt.scatter(X[:, 3][y==2], X[:, 4][y==2], marker='+', label=iris.target_names[2])
plt.legend(loc='upper left')
plt.xlabel(iris.feature_names[2])
plt.ylabel(iris.feature_names[3])
plt.title('Iris Data Set')
plt.show()
```



3.3 Softmax Regression

对 y 进行独热编码，得到矩阵G。

In [6]:
```
def oneHotY(y):
    # m为样本数
    m = y.shape[0]
    # k为类别数
    k = len(np.unique(y))

    oneHotY = np.zeros((m, k))
    for i in range(k):
        oneHotY[:, i] = (y==i)

    return oneHotY
```

In [7]:
```
G = oneHotY(y)
G.shape
```

Out[7]: (150, 3)

In [8]:
```
def initializeWithZeros(X, y):
    k = len(np.unique(y))

    return np.zeros((k, X.shape[1]))
```

In [9]:
```
def probabilityMatrix(X, theta):
    expScore = np.exp(X @ theta.T)
    sumScore = np.sum(expScore, axis=1).reshape(-1, 1)

    return np.multiply(expScore, sumScore)
```

In [10]:
```
def computeCost(X, G, theta, l):
    P = probabilityMatrix(X, theta)
    return -np.mean(np.multiply(G, np.log(P))) + l * theta.sum()
```

In [11]:
```
def computeGradient(X, G, theta, l):
    m = X.shape[0]
    P = probabilityMatrix(X, theta)
    grad = -((G-P).T @ X) / m + l *theta

    return grad
```

In [12]:
```
def batchGradientDescent(X, G, theta, alpha, iters, l, printFlag=True):
    costs = np.zeros(iters)

    for i in range(iters):
        theta = theta - alpha * computeGradient(X, G, theta, l)
        costs[i] = computeCost(X, G, theta, l)

        if printFlag and i % 1000 == 0:
            print(costs[i])

    return theta, costs
```

In [13]:
```
def predict(X, theta):
    P = probabilityMatrix(X, theta)

    return np.argmax(P, axis=1).reshape(-1, 1)
```

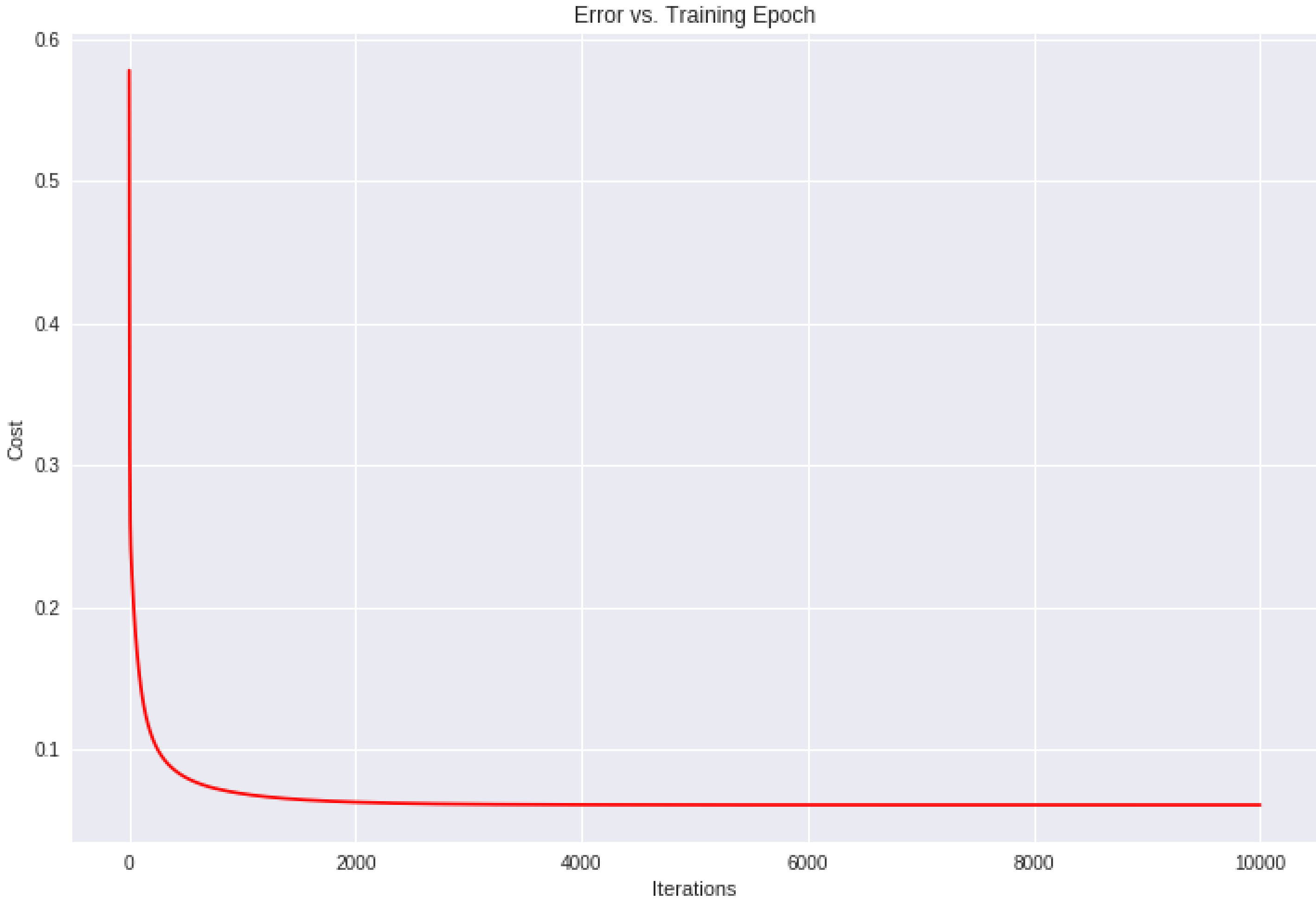
In [14]:
```
X, y = loadData(data)
G = oneHotY(y)
theta = initializeWithZeros(X, y)

iters = 10000
alpha = 0.01
l = 0.1

theta, costs = batchGradientDescent(X, G, theta, alpha, iters, l)
```

```
0.577650282651
0.0685942497214
0.062683569659
0.0612484292857
0.0608645968918
0.0607601270249
0.060731296824
0.0607232213633
0.0607209225948
0.0607202570216
```

In [15]:
```
plt.figure(figsize=(12, 8))
plt.plot(np.arange(iters), costs, color='red')
plt.xlabel('Iterations')
plt.ylabel('Cost')
plt.title('Error vs. Training Epoch')
plt.show()
```



In [16]:
```
y_pred = predict(X, theta)
print(classification_report(y, y_pred))
```

```
             precision    recall  f1-score   support

          0       1.00      1.00      1.00        50
          1       1.00      0.80      0.89        50
          2       0.83      1.00      0.91        50

avg / total       0.94      0.93      0.93       150
```

4. Softmax Regression 与 Logistic Regression 的关系

当类别数 $k=2$ 时，softmax regression 退化为 logistic regression。这表明 softmax regression 是 logistic regression 的一般形式。具体地说，当 $k=2$ 时，softmax regression 的假设函数为：

$$h_\theta(x) = \frac{1}{e^{\theta_1^T x} + e^{\theta_2^T x}} \begin{bmatrix} e^{\theta_1^T x} \\ e^{\theta_2^T x} \end{bmatrix}$$

利用 softmax regression 回归参数冗余的特点，我们令 $\psi = \theta_1$，并且从两个参数向量中都减去向量 θ_1，得到：

$$
\begin{aligned}
h(x) &= \frac{1}{e^{\vec{0}^T x} + e^{(\theta_2-\theta_1)^T x}} \begin{bmatrix} e^{\vec{0}^T x} \\ e^{(\theta_1-\theta_2)^T x} \end{bmatrix} \\
&= \begin{bmatrix} \frac{1}{1+e^{(\theta_1-\theta_2)^T x}} \\ \frac{e^{(\theta_1-\theta_2)^T x}}{1+e^{(\theta_1-\theta_2)^T x}} \end{bmatrix} \\
&= \begin{bmatrix} \frac{1}{1+e^{(\theta_1-\theta_2)^T x}} \\ 1 - \frac{1}{1+e^{(\theta_1-\theta_2)^T x}} \end{bmatrix}
\end{aligned}
$$

因此，用 θ' 来表示 $\theta_1 - \theta_2$，我们就会发现 softmax regression 预测其中一个类别的概率为 $\frac{1}{1+e^{(\theta')^T x}}$，另一个类别的概率为 $1 - \frac{1}{1+e^{(\theta')^T x}}$，这与logistic regression 是一致的。

5. Softmax Regression vs. k 个二元分类器

如果你在开发一个音乐分类的应用，需要对 k 种类型的音乐进行识别，那么是选择使用 softmax regression，还是使用 logistic regression 建立 k 个独立的二元分类器呢?

这一选择取决于你的类别之间是否互斥，例如，如果你有四个类别的音乐，分别为：古典音乐、乡村音乐、摇滚乐和爵士乐，那么你可以假设每个训练样本只会被打上一个标签（即一首歌只能属于这四种音乐类型的其中一种），此时，你应该使用类别数 $k = 4$ 的 softmax regression（如果在你的数据集中，有的歌曲不属于以上四类的其中任何一类，那么你可以添加一个"其他类"，并将类别数 k 设为5）。

如果你的四个类别如下：人声音乐、舞曲、影视原声、流行歌曲，那么这些类别之间并不是互斥的。例如：一首歌曲可以来源于影视原声，同时也包含人声。在这种情况下，使用4个二分类的 logistic regression 更为合适。这样每个新的音乐作品，我们的算法可以分别判断它是否属于各个类别。

现在，我们来看一个计算机视觉领域的例子，你的任务是将图像分到三个不同的类别中。（1）假设这三个类

别分别是：室内场景、户外城区场景、户外荒野场景。你会使用softmax regression 还是3个 logistic regression 呢？（2）现在假设这三个类别分别是室内场景、黑白图片、包含人物的图片，你会选择 softmax regression 还是多个 logistic regression 呢?

在第一个例子中，三个类别是互斥的，因此，更适于选择 softmax regression。而在第二个例子中，建立三个独立的 logistic regression 更加合适。

In [ ]:
```

```