SoftmaxRegression: Multiclass version of logistic regression

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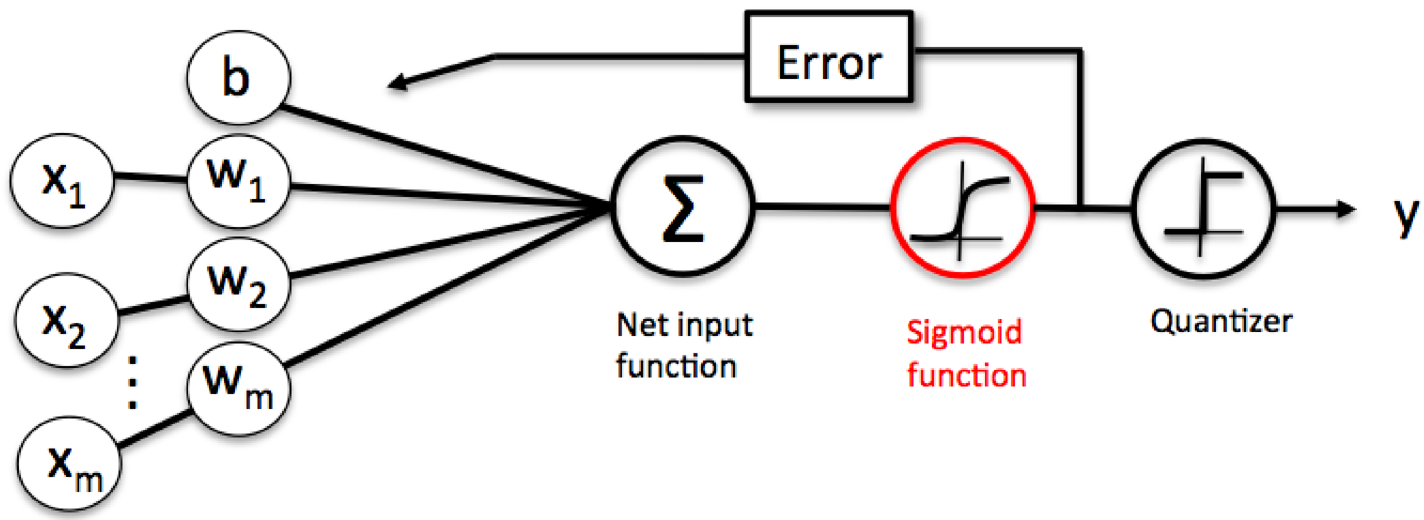
A logistic regression class for multi-class classification tasks.

```
from mlxtend.classifier import SoftmaxRegression
```

Overview

Softmax Regression (synonyms: *Multinomial Logistic*, *Maximum Entropy Classifier*, or just *Multi-class Logistic Regression*) is a generalization of logistic regression that we can use for multi-class classification (under the assumption that the classes are mutually exclusive). In contrast, we use the (standard) *Logistic Regression* model in binary classification tasks.

Below is a schematic of a *Logistic Regression* model, for more details, please see the `LogisticRegression` manual.



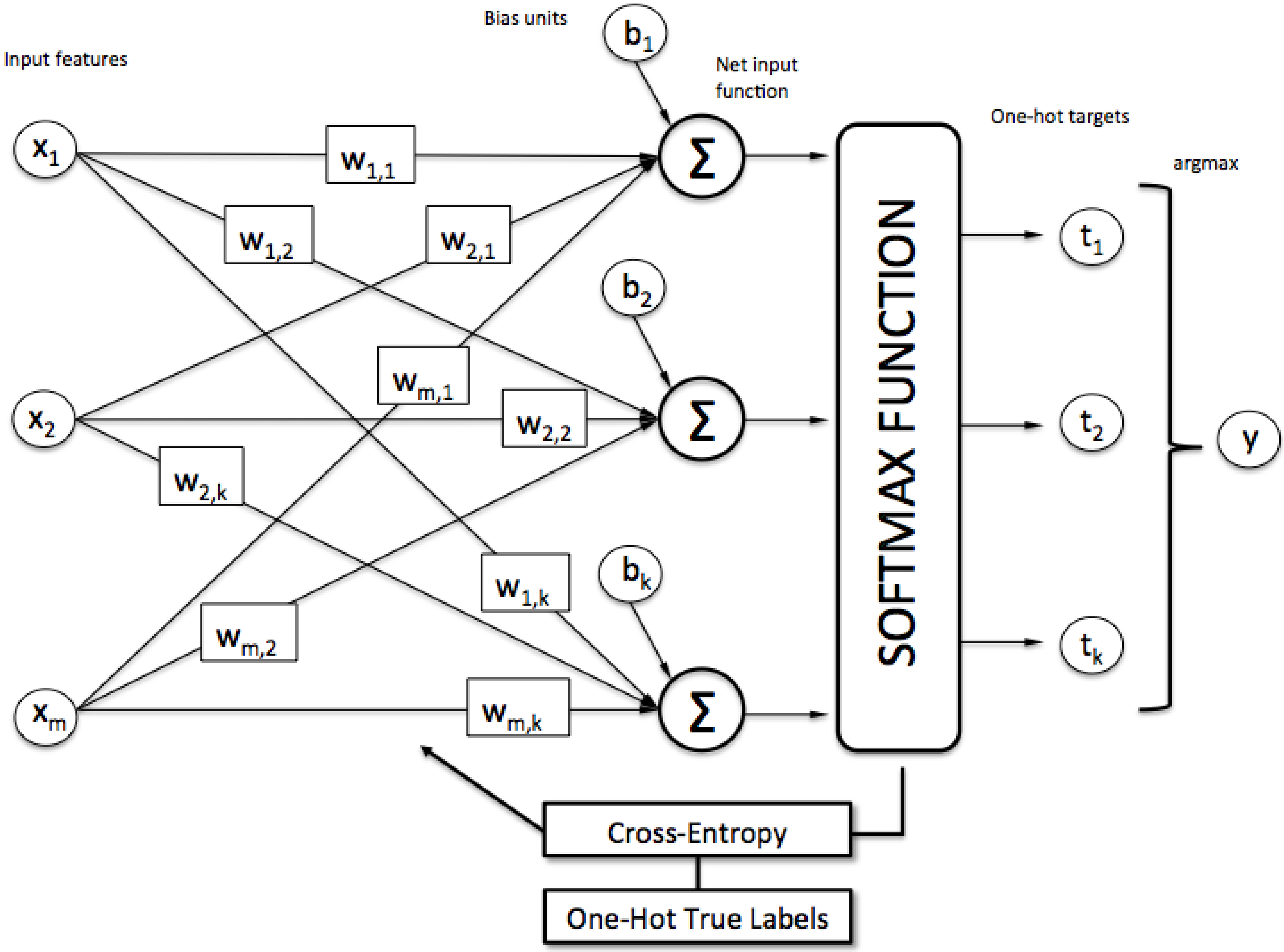
In *Softmax Regression* (SMR), we replace the sigmoid logistic function by the so-called *softmax* function $\phi_{softmax}(\cdot)$.

$$P(y = j \mid z^{(i)}) = \phi_{softmax}(z^{(i)}) = \frac{e^{z^{(i)}}}{\sum_{j=0}^{k} e^{z_{k}^{(i)}}},$$

where we define the net input *z* as

$$z = w_1 x_1 + \ldots + w_m x_m + b = \sum_{l=1}^{m} w_l x_l + b = \mathbf{w}^T \mathbf{x} + b.$$

($\mathbf{w}$ is the weight vector, $\mathbf{x}$ is the feature vector of 1 training sample, and b is the bias unit.)
Now, this softmax function computes the probability that this training sample $\mathbf{x}^{(i)}$ belongs to class j given the weight and net input $z^{(i)}$. So, we compute the probability $p(y = j \mid \mathbf{x^{(i)}; w}_j)$ for each class label in $j = 1, \ldots, k.$. Note the normalization term in the denominator which causes these class probabilities to sum up to one.



To illustrate the concept of softmax, let us walk through a concrete example. Let's assume we have a training set consisting of 4 samples from 3 different classes (0, 1, and 2)

- $x_0 \rightarrow \text{class } 0$
- $x_1 \rightarrow \text{class } 1$
- $x_2 \rightarrow \text{class } 2$
- $x_3 \rightarrow \text{class } 2$

```
import numpy as np
```

```
y = np.array([0, 1, 2, 2])
```

First, we want to encode the class labels into a format that we can more easily work with; we apply one-hot encoding:

```
y_enc = (np.arange(np.max(y) + 1) == y[:, None]).astype(float)

print('one-hot encoding:\n', y_enc)

one-hot encoding:
 [[ 1.  0.  0.]
 [ 0.  1.  0.]
 [ 0.  0.  1.]
 [ 0.  0.  1.]]
```

A sample that belongs to class 0 (the first row) has a 1 in the first cell, a sample that belongs to class 2 has a 1 in the second cell of its row, and so forth.

Next, let us define the feature matrix of our 4 training samples. Here, we assume that our dataset consists of 2 features; thus, we create a 4x2 dimensional matrix of our samples and features. Similarly, we create a 2x3 dimensional weight matrix (one row per feature and one column for each class).

```
X = np.array([[0.1, 0.5],
              [1.1, 2.3],
              [-1.1, -2.3],
              [-1.5, -2.5]])
```

```
W = np.array([[0.1, 0.2, 0.3],
              [0.1, 0.2, 0.3]])

bias = np.array([0.01, 0.1, 0.1])

print('Inputs X:\n', X)
print('\nWeights W:\n', W)
print('\nbias:\n', bias)
```

```
Inputs X:
 [[ 0.1  0.5]
 [ 1.1  2.3]
 [-1.1 -2.3]
 [-1.5 -2.5]]

Weights W:
 [[ 0.1  0.2  0.3]
 [ 0.1  0.2  0.3]]

bias:
 [ 0.01  0.1   0.1 ]
```

To compute the net input, we multiply the 4x2 matrix feature matrix `X` with the 2x3 (n_features x n_classes) weight matrix `W`, which yields a 4x3 output matrix (n_samples x n_classes) to which we then add the bias unit:

$$\mathbf{Z} = \mathbf{X}\mathbf{W} + \mathbf{b}.$$

```
X = np.array([[0.1, 0.5],
              [1.1, 2.3],
              [-1.1, -2.3],
              [-1.5, -2.5]])

W = np.array([[0.1, 0.2, 0.3],
              [0.1, 0.2, 0.3]])

bias = np.array([0.01, 0.1, 0.1])

print('Inputs X:\n', X)
print('\nWeights W:\n', W)
print('\nbias:\n', bias)
```

```
Inputs X:
 [[ 0.1  0.5]
 [ 1.1  2.3]
 [-1.1 -2.3]
 [-1.5 -2.5]]

Weights W:
 [[ 0.1  0.2  0.3]
 [ 0.1  0.2  0.3]]

bias:
 [ 0.01  0.1   0.1 ]
```

```
def net_input(X, W, b):
    return (X.dot(W) + b)

net_in = net_input(X, W, bias)
print('net input:\n', net_in)
```

```
net input:
 [[ 0.07  0.22  0.28]
 [ 0.35  0.78  1.12]
 [-0.33 -0.58 -0.92]
 [-0.39 -0.7  -1.1 ]]
```

Now, it's time to compute the softmax activation that we discussed earlier:

$$P(y = j \mid z^{(i)}) = \phi_{softmax}(z^{(i)}) = \frac{e^{z^{(i)}}}{\sum_{j=0}^{k} e^{z_k^{(i)}}}.$$

```
def softmax(z):
    return (np.exp(z.T) / np.sum(np.exp(z), axis=1)).T

smax = softmax(net_in)
print('softmax:\n', smax)
```

```
softmax:
 [[ 0.29450637  0.34216758  0.36332605]
 [ 0.21290077  0.32728332  0.45981591]
```

```
 [ 0.42860913  0.33380113  0.23758974]
 [ 0.44941979  0.32962558  0.22095463]]
```

As we can see, the values for each sample (row) nicely sum up to 1 now. E.g., we can say that the first sample `[ 0.29450637 0.34216758 0.36332605]` has a 29.45% probability to belong to class 0.

Now, in order to turn these probabilities back into class labels, we could simply take the argmax-index position of each row:

[[0.29450637 0.34216758 **0.36332605**] -> 2
[0.21290077 0.32728332 **0.45981591**] -> 2
[**0.42860913** 0.33380113 0.23758974] -> 0
[**0.44941979** 0.32962558 0.22095463]] -> 0

```
def to_classlabel(z):
    return z.argmax(axis=1)

print('predicted class labels: ', to_classlabel(smax))
```

```
predicted class labels:  [2 2 0 0]
```

As we can see, our predictions are terribly wrong, since the correct class labels are `[0, 1, 2, 2]`. Now, in order to train our logistic model (e.g., via an optimization algorithm such as gradient descent), we need to define a cost function $J(\cdot)$ that we want to minimize:

$$J(\mathbf{W}; \mathbf{b}) = \frac{1}{n} \sum_{i=1}^{n} H(T_i, O_i),$$

which is the average of all cross-entropies over our n training samples. The cross-entropy function is defined as

$$H(T_i, O_i) = -\sum_{m} T_i \cdot log(O_i).$$

Here the T stands for "target" (i.e., the *true* class labels) and the O stands for output -- the computed *probability* via softmax; **not** the predicted class label.

```
def cross_entropy(output, y_target):
    return - np.sum(np.log(output) * (y_target), axis=1)


xent = cross_entropy(smax, y_enc)
print('Cross Entropy:', xent)
```

```
Cross Entropy: [ 1.22245465 1.11692907 1.43720989
1.50979788]
```

```
def cost(output, y_target):
    return np.mean(cross_entropy(output, y_target))


J_cost = cost(smax, y_enc)
print('Cost: ', J_cost)
```

```
Cost:  1.32159787159
```

In order to learn our softmax model -- determining the weight coefficients -- via gradient descent, we then need to compute the derivative

$$\nabla \mathbf{w}_j \, J(\mathbf{W}; \mathbf{b}).$$

I don't want to walk through the tedious details here, but this cost derivative turns out to be simply:

$$\nabla \mathbf{w}_j \, J(\mathbf{W}; \mathbf{b}) = \frac{1}{n} \sum_{i=0}^{n} \big[\mathbf{x}^{(i)} \, \big(O_i - T_i\big) \big]$$

We can then use the cost derivate to update the weights in opposite direction of the cost gradient with learning rate η:

$$\mathbf{w}_j := \mathbf{w}_j - \eta \nabla \mathbf{w}_j \, J(\mathbf{W}; \mathbf{b})$$

for each class

$$j \in \{0, 1, \ldots, k\}$$

(note that $\mathbf{w}_j$ is the weight vector for the class $y = j$), and we update the bias units

$$\mathbf{b}_j := \mathbf{b}_j - \eta \bigg[\frac{1}{n} \sum_{i=0}^{n} \big(O_i - T_i\big) \bigg].$$

As a penalty against complexity, an approach to reduce the variance of our model and decrease the degree of overfitting by adding additional bias, we can further add a regularization term such as the L2 term with the regularization parameter λ:

L2: $\frac{\lambda}{2}||\mathbf{w}||_2^2$,

where

$$||\mathbf{w}||_2^2 = \sum_{l=0}^{m} \sum_{j=0}^{k} w_{i,j}$$

so that our cost function becomes

$$J(\mathbf{W}; \mathbf{b}) = \frac{1}{n} \sum_{i=1}^{n} H(T_i, O_i) + \frac{\lambda}{2}||\mathbf{w}||_2^2$$

and we define the "regularized" weight update as

$$\mathbf{w}_j := \mathbf{w}_j - \eta \big[\nabla \mathbf{w}_j \, J(\mathbf{W}) + \lambda \mathbf{w}_j\big].$$

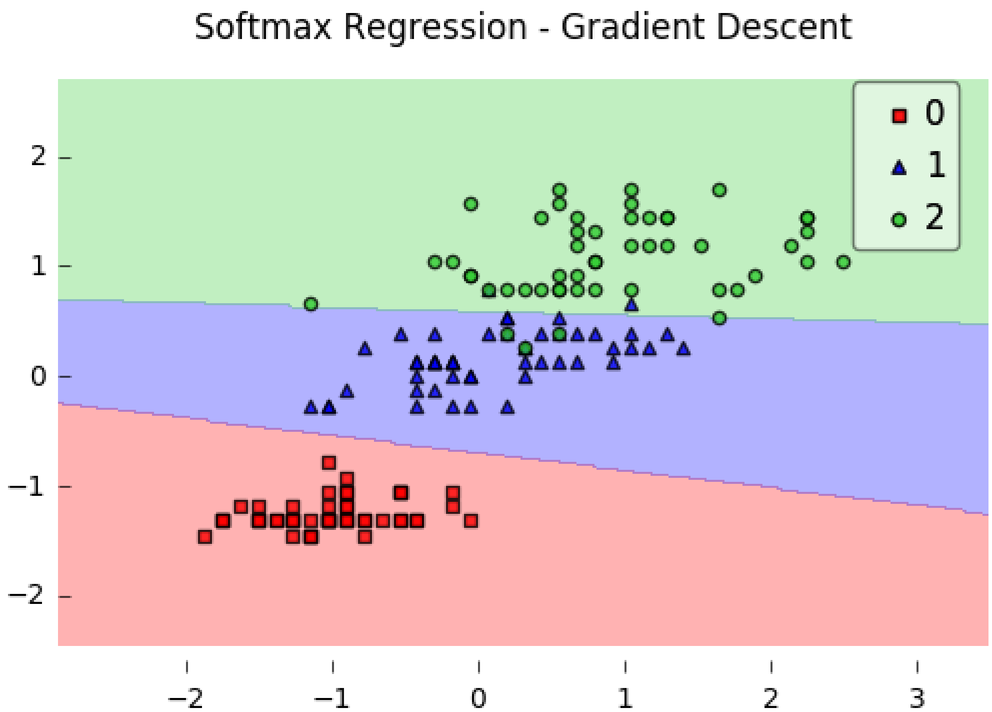
(Please note that we don't regularize the bias term.)

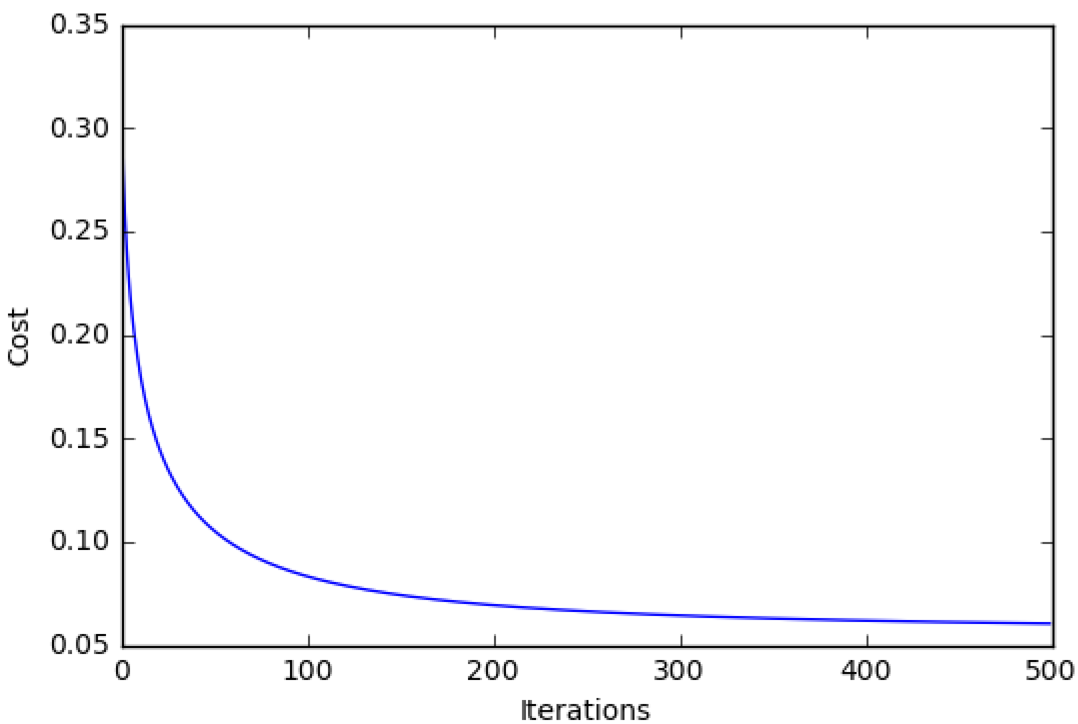
Example 1 - Gradient Descent

```
from mlxtend.data import iris_data
from mlxtend.plotting import plot_decision_regions
from mlxtend.classifier import SoftmaxRegression
import matplotlib.pyplot as plt

# Loading Data

X, y = iris_data()
X = X[:, [0, 3]] # sepal length and petal width
```

```
# standardize
X[:,0] = (X[:,0] - X[:,0].mean()) / X[:,0].std()
X[:,1] = (X[:,1] - X[:,1].mean()) / X[:,1].std()

lr = SoftmaxRegression(eta=0.01,
                       epochs=500,
                       minibatches=1,
                       random_seed=1,
                       print_progress=3)
lr.fit(X, y)

plot_decision_regions(X, y, clf=lr)
plt.title('Softmax Regression - Gradient Descent')
plt.show()

plt.plot(range(len(lr.cost_)), lr.cost_)
plt.xlabel('Iterations')
plt.ylabel('Cost')
plt.show()
```

```
Iteration: 500/500 | Cost 0.06 | Elapsed: 0:00:00 | ETA:
0:00:00
```





Predicting Class Labels

```
y_pred = lr.predict(X)
print('Last 3 Class Labels: %s' % y_pred[-3:])
```

```
Last 3 Class Labels: [2 2 2]
```

Predicting Class Probabilities

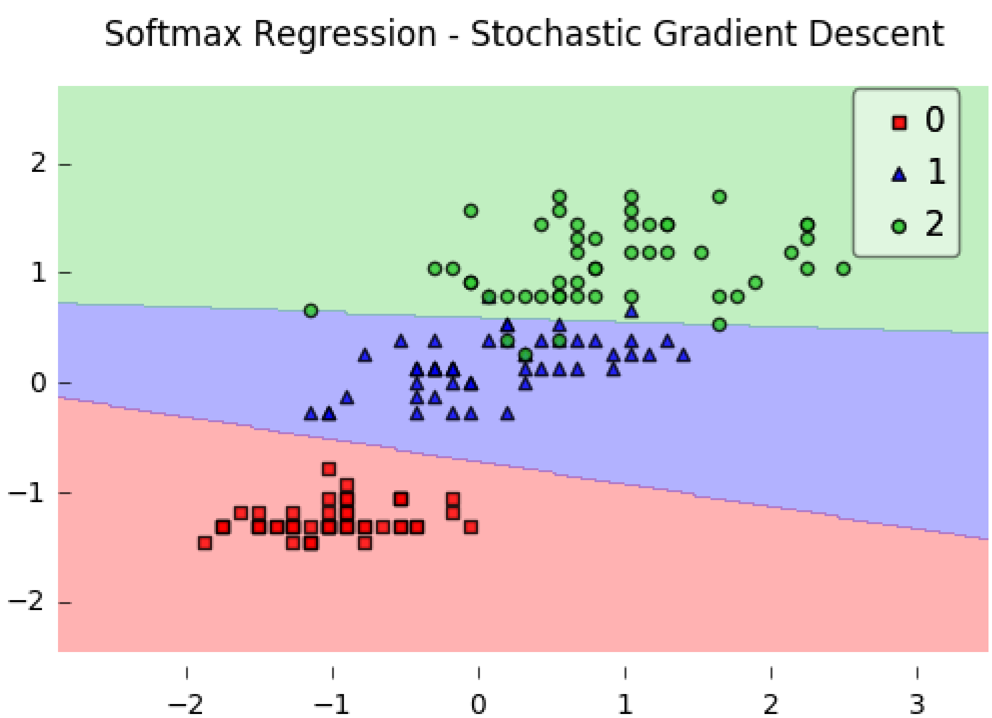
```
y_pred = lr.predict_proba(X)
print('Last 3 Class Labels:\n %s' % y_pred[-3:])
```

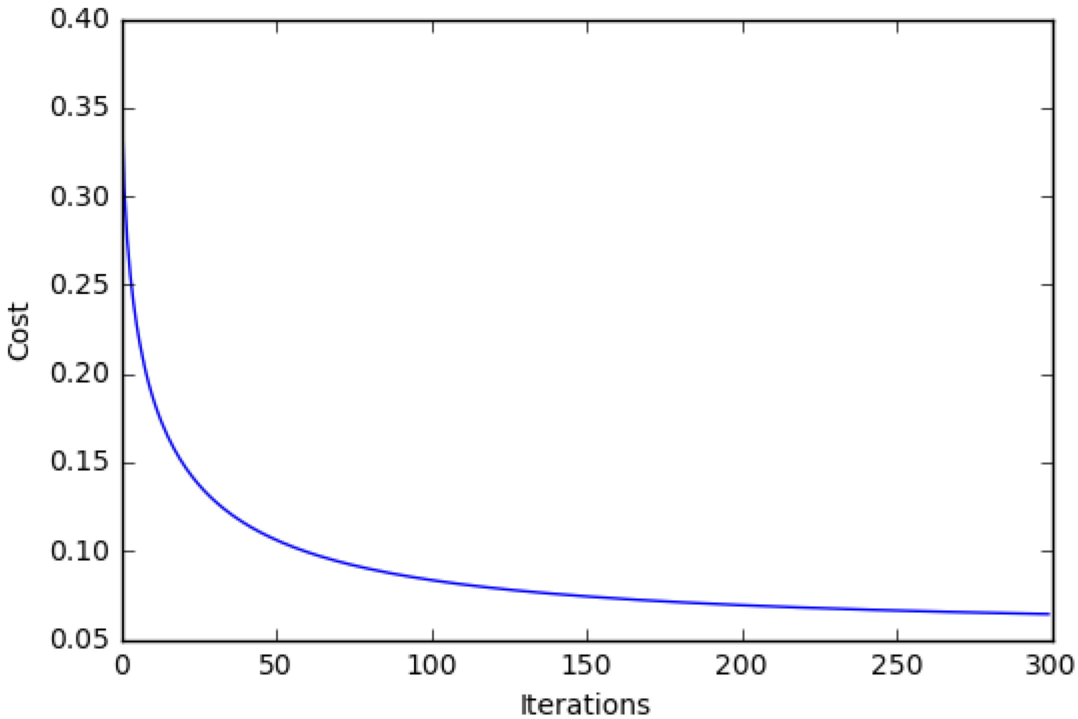
```
Last 3 Class Labels:
 [[  9.18728149e-09   1.68894679e-02   9.83110523e-01]
 [  2.97052325e-11   7.26356627e-04   9.99273643e-01]
 [  1.57464093e-06   1.57779528e-01   8.42218897e-01]]
```

Example 2 - Stochastic Gradient Descent

```
from mlxtend.data import iris_data
from mlxtend.plotting import plot_decision_regions
from mlxtend.classifier import SoftmaxRegression
import matplotlib.pyplot as plt

# Loading Data

X, y = iris_data()
X = X[:, [0, 3]] # sepal length and petal width

# standardize
X[:,0] = (X[:,0] - X[:,0].mean()) / X[:,0].std()
X[:,1] = (X[:,1] - X[:,1].mean()) / X[:,1].std()
```

```
lr = SoftmaxRegression(eta=0.01, epochs=300, minibatches=len(y), random_seed=1)
lr.fit(X, y)

plot_decision_regions(X, y, clf=lr)
plt.title('Softmax Regression - Stochastic Gradient Descent')
plt.show()

plt.plot(range(len(lr.cost_)), lr.cost_)
plt.xlabel('Iterations')
plt.ylabel('Cost')
plt.show()
```





API

SoftmaxRegression(eta=0.01, epochs=50, l2=0.0, minibatches=1, n_classes=None, random_seed=None, print_progress=0)

Softmax regression classifier.

Parameters

- `eta` : float (default: 0.01)

  Learning rate (between 0.0 and 1.0)

- `epochs` : int (default: 50)

  Passes over the training dataset. Prior to each epoch, the dataset is shuffled if `minibatches > 1` to prevent cycles in stochastic gradient descent.

- `l2` : float

  Regularization parameter for L2 regularization. No regularization if l2=0.0.

- `minibatches` : int (default: 1)

  The number of minibatches for gradient-based optimization. If 1: Gradient Descent learning If len(y): Stochastic Gradient Descent (SGD) online learning If 1 < minibatches < len(y): SGD Minibatch learning

- `n_classes` : int (default: None)

  A positive integer to declare the number of class labels if not all class labels are present in a partial training set. Gets the number of class labels automatically if None.

- `random_seed` : int (default: None)

  Set random state for shuffling and initializing the weights.

- `print_progress` : int (default: 0)

  Prints progress in fitting to stderr. 0: No output 1: Epochs elapsed and cost 2: 1 plus time elapsed 3: 2 plus estimated time until completion

Attributes

- `w_` : 2d-array, shape={n_features, 1}

Model weights after fitting.

- `b_` : 1d-array, shape={1,}

  Bias unit after fitting.

- `cost_` : list

  List of floats, the average cross_entropy for each epoch.

Examples

For usage examples, please see http://rasbt.github.io/mlxtend/user_guide/classifier/SoftmaxRegression/

Methods

fit(X, y, init_params=True)

Learn model from training data.

Parameters

- `X` : {array-like, sparse matrix}, shape = [n_samples, n_features]

  Training vectors, where n_samples is the number of samples and n_features is the number of features.

- `y` : array-like, shape = [n_samples]

  Target values.

- `init_params` : bool (default: True)

  Re-initializes model parameters prior to fitting. Set False to continue training with weights from a previous model fitting.

Returns

- `self` : object

predict(X)

Predict targets from X.

Parameters

- `X` : {array-like, sparse matrix}, shape = [n_samples, n_features]

  Training vectors, where n_samples is the number of samples and n_features is the number of features.

Returns

- `target_values` : array-like, shape = [n_samples]

  Predicted target values.

predict_proba(X)

Predict class probabilities of X from the net input.

Parameters

- `X` : {array-like, sparse matrix}, shape = [n_samples, n_features]

  Training vectors, where n_samples is the number of samples and n_features is the number of features.

Returns

- `Class probabilties` : array-like, shape= [n_samples, n_classes]

score(X, y)

Compute the prediction accuracy

Parameters

- `X` : {array-like, sparse matrix}, shape = [n_samples, n_features]

  Training vectors, where n_samples is the number of samples and n_features is the number of features.

- `y` : array-like, shape = [n_samples]

  Target values (true class labels).

Returns

- `acc` : float

  The prediction accuracy as a float between 0.0 and 1.0 (perfect score).

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