Perceptron, Adaline, and Optimization

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```python
In [1]:   # inline plotting instead of popping out
          %matplotlib inline

          import os, math
          from IPython.display import Image
          import numpy as np
          seed = np.random.seed

          import pandas as pd
          import matplotlib.pyplot as plt

          from sklearn.linear_model import Perceptron
          from sklearn.metrics import accuracy_score
          from sklearn.model_selection import train_test_split
          from sklearn.preprocessing import StandardScaler
```

```python
In [2]:   # load utility classes/functions e.g., plot_decision_regions()
          import urllib.request

          urllib.request.urlretrieve("https://nthu-datalab.github.io/ml/labs/04-1_Perceptron_Adaline/lab04lib.py",

          from lab04lib import *
```

In this lab, we will guide you through the implementation of Perceptron and Adaline, two of the first algorithmically described machine learning algorithms for the classification problem. We will also discuss how to train these models using the optimization techniques, including the gradient descent (GD) and stochastic gradient descent (SGD), and compare their convergence speed.

Data Preparation

We use the Iris dataset from the UCI machine learning repository, which is one of the best known datasets in classification. It consists of 150 iris plants as examples, each with the sepal and petal sizes as attributes and the type as class label. Let's download the Iris dataset using Pandas first:

```python
In [3]:   df = pd.read_csv(
              'https://archive.ics.uci.edu/ml/'
              'machine-learning-databases/iris/iris.data',
              header = None
          )
          df.columns = ['Sepal length', 'Sepal width', 'Petal length', 'Petal width', 'Class label']
          display(df.head())

          X = df[['Petal length', 'Petal width']].values
          y = pd.factorize(df['Class label'])[0]

          X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, random_state=0)

          print('# Training data points: {}'.format(X_train.shape[0]))
          print('# Testing data points: {}'.format(X_test.shape[0]))
          print('Class labels: {} (mapped from {}'.format(np.unique(y), np.unique(df['Class label'])))
```

	Sepal length	Sepal width	Petal length	Petal width	Class label
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

```
# Training data points: 100
# Testing data points: 50
Class labels: [0 1 2] (mapped from ['Iris-setosa' 'Iris-versicolor' 'Iris-virginica']
```

Standardization for Gradient Descent

Recall from the lecture that the gradient descent may perform poorly if the Hessian of the function f to be minimized has a large condition number. In this case, the surface of f can be curvy in some directions but flat in the others. Therefore, the gradient descent, which ignores the curvatures, may overshoot the optimal point along curvy directions but take too small step along flat ones.

One common way to improve the conditioning of f is to standardize dataset X, as follows:

In [4]:
```python
sc = StandardScaler()
sc.fit(X_train)
X_train_std = sc.transform(X_train)
X_test_std = sc.transform(X_test)
```

Note: the standardization should calculate the mean μ and variance σ^2 using only the training set, as the testing set must be remain unknown during the entire training process.

Training Perceptron via Scikit-learn

Having standardized the training data, we can now train a Perceptron model:

In [5]:
```python
# max_iter : The maximum number of passes over the training data
# eta0 : learning rate
ppn = Perceptron(max_iter=10, eta0=0.1, random_state=0)
ppn.fit(X_train_std, y_train)
```

Out[5]:
```
▼           Perceptron
Perceptron(eta0=0.1, max_iter=10)
```

Having trained a model in Scikit-learn, we can make predictions over the testing set and report the accuracy. Note that the testing set should be standardized in the exact same way as the training set.

In [6]:
```python
y_pred = ppn.predict(X_test_std)
print('Misclassified samples: %d' % (y_test != y_pred).sum())
print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))
```

```
Misclassified samples: 5
Accuracy: 0.90
```

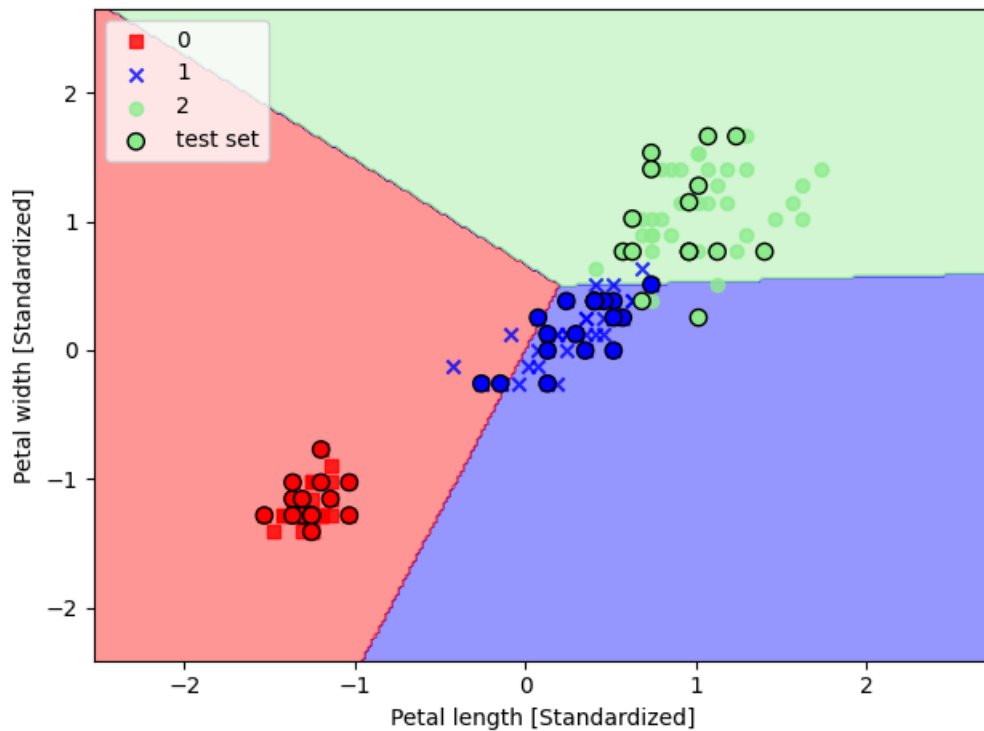We get 90% accuracy. Now let's plot the decision boundaries to see how the model works:

In [7]:
```python
if not os.path.exists('./output'):
    os.makedirs('./output')

X_combined_std = np.vstack((X_train_std, X_test_std))
y_combined = np.hstack((y_train, y_test))

plot_decision_regions(X=X_combined_std, y=y_combined,
                      classifier=ppn, test_idx=range(len(y_train),
                                                     len(y_train) + len(y_test)))
plt.xlabel('Petal length [Standardized]')
plt.ylabel('Petal width [Standardized]')
plt.legend(loc='upper left')

plt.tight_layout()
plt.savefig('./output/fig-perceptron-scikit.png', dpi=300)
plt.show()
```

Multiclass Classification

The Perceptron model is originally designed for the binary classification problems. However, we can see from the above that the model implemented in the Scikit-learn is able to predict the labels of multiple classes (3 in this case). This is achieved by wrapping the binary model with an **One-vs-All** (or **One-vs-Rest**) procedure. If there are K classes, then this procedure trains K binary classifiers for each class, where each classifier treats only one class as positive and the rests as negative. To predict the label of a testing data point, each classifier generates the soft output $f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} - b \in \mathbb{R}$ for every class, and then the class who gets the highest output value becomes the predicted label.

Implementing Perceptron

Now it's time to implement a classifier by our own. For simplicity, we only implement the binary Perceptron model. This can be easily done as follows:

```python
class Perceptron2(object):
    """Perceptron classifier.

    Parameters
    ------------
    eta: float
        Learning rate (between 0.0 and 1.0)
    n_iter: int
        Number of epochs, i.e., passes over the training dataset.

    Attributes
    ------------
    w_: 1d-array
        Weights after fitting.
    errors_: list
        Number of misclassifications in every epoch.
    random_state : int
        The seed of the pseudo random number generator.
    """

    def __init__(self, eta=0.01, n_iter=10, random_state=1):
        self.eta = eta
        self.n_iter = n_iter
        self.random_state = random_state

    def fit(self, X, y):
```

```
        """Fit training data.

        Parameters
        ----------
        X : array-like; 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, or labels.

        Returns
        -------
        self : object

        """
        rgen = np.random.RandomState(self.random_state)
        self.w_ = rgen.normal(loc=0.0, scale=0.01, size=1+X.shape[1])
        self.errors_ = []

        for _ in range(self.n_iter):
            errors = 0.0
            for xi, yi in zip(X, y):
                output = self.predict(xi)
                error = (yi - output)
                self.w_[1:] += self.eta * error * xi
                self.w_[0] += self.eta * error
                errors += int(error != 0.0)
            self.errors_.append(errors)
        return self

    def net_input(self, X):
        """Calculate net input"""
        return np.dot(X, self.w_[1:]) + self.w_[0]

    def predict(self, X):
        """Return class label after unit step"""
        return np.where(self.net_input(X) >= 0.0, 1, -1)
```

NOTE:

1. we could have implemented the shorthand version of X and w to include the bias term. However, we single out the addition of the bias term (`self.w_[0]`) for performance reason, as adding a vector of 1's to the training array each time we want to make a prediction would be inefficient.
2. some production implementation shuffles data in the beginning of each epoch. We omit this step for simplicity.

To train our binary Perceptron model using the Iris dataset, we recreate our training and testing sets so that they contain only binary labels:

```
In [9]:  # discard exmaples in the first class
         X = X[50:150]
         y = np.where(y[50:150] == 2, -1, y[50:150])

         X_train, X_test, y_train, y_test = train_test_split(
             X, y, test_size=0.1, random_state=1)

         sc = StandardScaler()
         sc.fit(X_train)
         X_train_std = sc.transform(X_train)
         X_test_std = sc.transform(X_test)

         print('# Training data points: %d' % X_train.shape[0])
         print('# Testing data points: %d' % X_test.shape[0])
         print('Class labels: %s' % np.unique(y))
```

```
# Training data points: 90
# Testing data points: 10
Class labels: [-1  1]
```

Let's train our model:

In [10]:
```python
# training

ppn2 = Perceptron2(eta=0.1, n_iter=20)

ppn2.fit(X_train_std, y_train)

# testing

y_pred = ppn2.predict(X_test_std)
print('Misclassified samples: %d' % (y_test != y_pred).sum())
print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))

# plot descision boundary

X_combined_std = np.vstack((X_train_std, X_test_std))
y_combined = np.hstack((y_train, y_test))

plot_decision_regions(X=X_combined_std, y=y_combined,
                      classifier=ppn2, test_idx=range(len(y_train),
                                                      len(y_train) + len(y_test)))
plt.xlabel('Petal length [Standardized]')
plt.ylabel('Petal width [Standardized]')
plt.legend(loc='upper left')
plt.tight_layout()
plt.savefig('./output/fig-perceptron2-boundary.png', dpi=300)
plt.show()
```
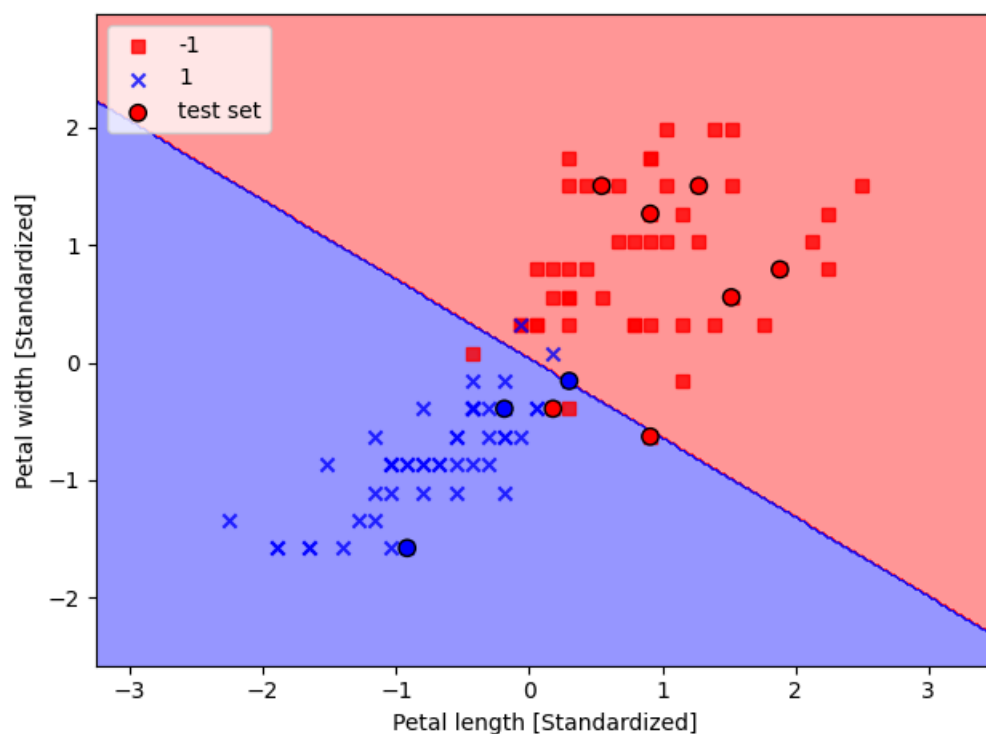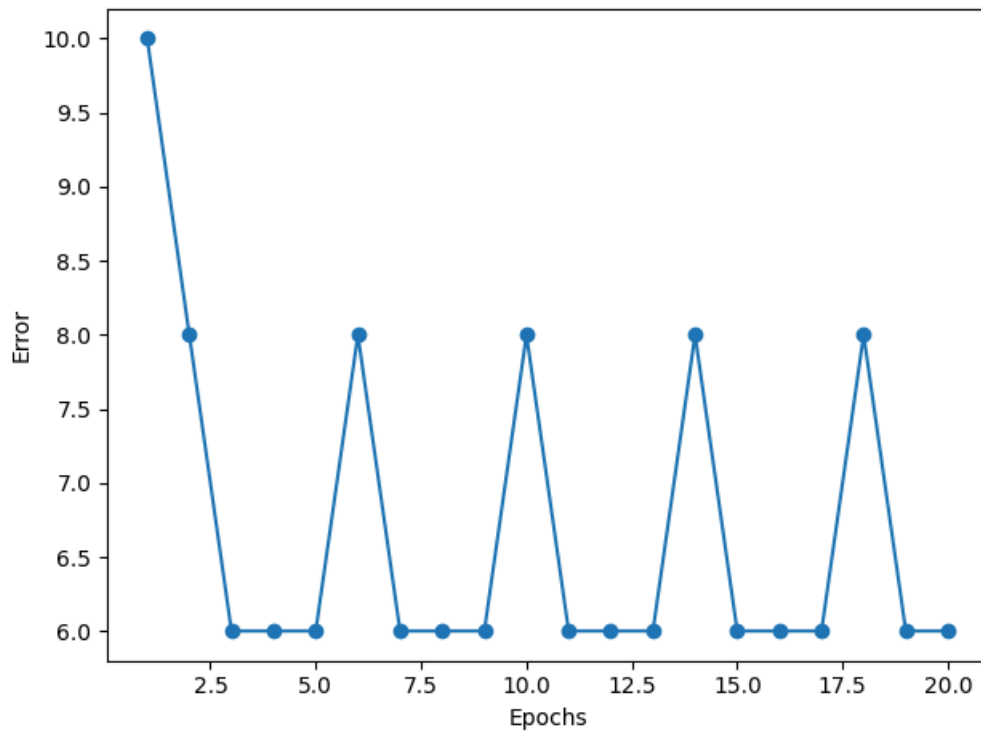
```
Misclassified samples: 3
Accuracy: 0.70
```


Our Perceptron model achieves 70% accuracy, which is not too good. This is mainly because the training algorithm does not converge when the data points are **not** linearly separable (by a hyperplane). We can track convergence using the `errors_` attributes:

In [11]:
```python
plt.plot(range(1, len(ppn2.errors_) + 1), ppn2.errors_, marker='o')
plt.xlabel('Epochs')
plt.ylabel('Error')

plt.tight_layout()
plt.savefig('./output/fig-perceptron2_errors.png', dpi=300)
plt.show()
```

As we can see, the weights never stop updating. To terminate the training process, we have to set a maximum number of epochs.

Implementing Adaline with GD

The ADAptive LInear NEuron (Adaline) is similar to the Perceptron, except that it defines a cost function based on the soft output and an optimization problem. We can therefore leverage various optimization techniques to train Adaline in a more theoretic grounded manner. Let's implement the Adaline using the batch gradient descent (GD) algorithm:

```python
In [12]:
class AdalineGD(object):
    """ADAptive LInear NEuron classifier.

    Parameters
    ------------
    eta : float
        Learning rate (between 0.0 and 1.0)
    n_iter : int
        Passes over the training dataset.
    random_state : int
        The seed of the pseudo random number generator.

    Attributes
    -----------
    w_ : 1d-array
        Weights after fitting.
    errors_ : list
        Number of misclassifications in every epoch.

    """
    def __init__(self, eta=0.01, n_iter=50, random_state=1):
        self.eta = eta
        self.n_iter = n_iter
        self.random_state = random_state

    def fit(self, X, y):
        """ Fit training data.

        Parameters
        ----------
        X : array-like; 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 or labels.

        Returns
        -------
        self : object

        """
        rgen = np.random.RandomState(self.random_state)
        self.w_ = rgen.normal(loc=0.0, scale=0.01, size=1+X.shape[1])
        self.cost_ = []

        for i in range(self.n_iter):
            output = self.activation(X)

            # Cost function
            error = (y - output)
            cost = (error**2).sum() / 2.0
            self.cost_.append(cost)

            # Update rule
            self.w_[1:] += self.eta * X.T.dot(error)
            self.w_[0] += self.eta * error.sum()

        return self

    def net_input(self, X):
        """Calculate net input"""
        return np.dot(X, self.w_[1:]) + self.w_[0]

    def activation(self, X):
        """Compute linear activation"""
        return self.net_input(X)

    def predict(self, X):
        """Return class label after unit step"""
        return np.where(self.activation(X) >= 0.0, 1, -1)
```

As discussed in the lecture, a good learning rate η is a key to the optimal convergence. In practice, it often requires some experimentation to find a good learning rate. Let's plot the cost against the number of epochs for the two different learning rates:
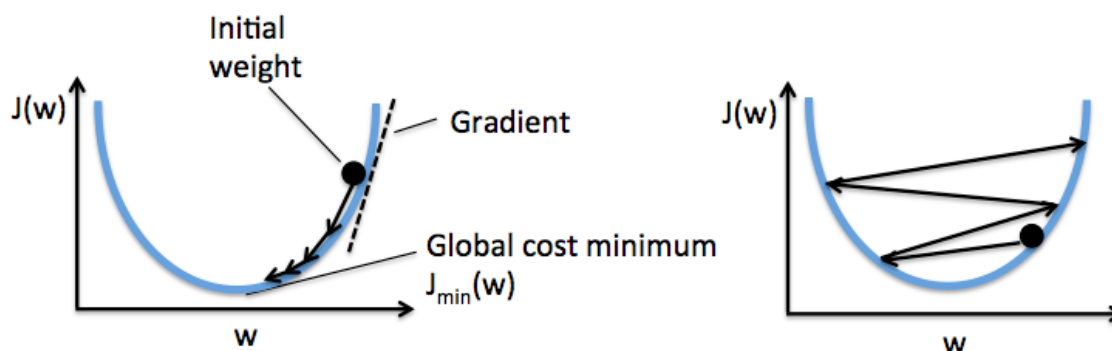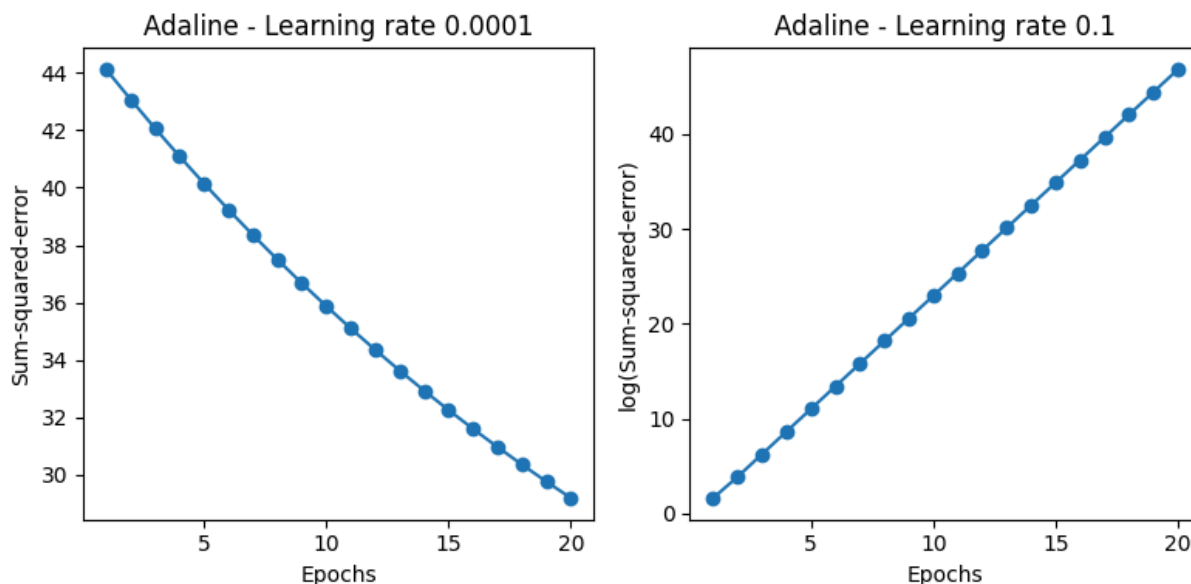
```
In [13]: fig, ax = plt.subplots(nrows=1, ncols=2, figsize=(8, 4))

ada1 = AdalineGD(n_iter=20, eta=0.0001).fit(X_train_std, y_train)
ax[0].plot(range(1, len(ada1.cost_) + 1), ada1.cost_, marker='o')
ax[0].set_xlabel('Epochs')
ax[0].set_ylabel('Sum-squared-error')
ax[0].set_title('Adaline - Learning rate 0.0001')

ada2 = AdalineGD(n_iter=20, eta=0.1).fit(X_train_std, y_train)
ax[1].plot(range(1, len(ada2.cost_) + 1), np.log10(ada2.cost_), marker='o')
ax[1].set_xlabel('Epochs')
ax[1].set_ylabel('log(Sum-squared-error)')
ax[1].set_title('Adaline - Learning rate 0.1')

plt.tight_layout()
plt.savefig('./output/fig-adaline-gd-overshoot.png', dpi=300)
plt.show()
```

The left figure shows what could happen if we choose a too small learning rate: although the cost decreases, the descent is too small that the algorithm would require a **large number of epochs** to converge. On the other hand, the right figure shows what could happen if we choose a learning rate that is too large: instead of minimizing the cost function, the error becomes larger in every epoch because we **overshoot** the optimal point every time. This is illustrated below:

With a properly chosen learning rate η, the AdalineGD converges and gives a better prediction accuracy (80%) as compared with the Perceptron (70%):

```
In [14]:  ada = AdalineGD(n_iter=20, eta=0.01)
          ada.fit(X_train_std, y_train)

          # cost values

          plt.plot(range(1, len(ada.cost_) + 1), ada.cost_, marker='o')
          plt.xlabel('Epochs')
          plt.ylabel('Sum-squared-error')

          plt.tight_layout()
          plt.savefig('./output/fig-adalin-gd-cost.png', dpi=300)
          plt.show()

          # testing accuracy

          y_pred = ada.predict(X_test_std)
          print('Misclassified samples: %d' % (y_test != y_pred).sum())
          print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))

          # plot decision boundary

          plot_decision_regions(X_combined_std, y_combined,
                                classifier=ada, test_idx=range(len(y_train),
                                                               len(y_train) + len(y_test)))
```
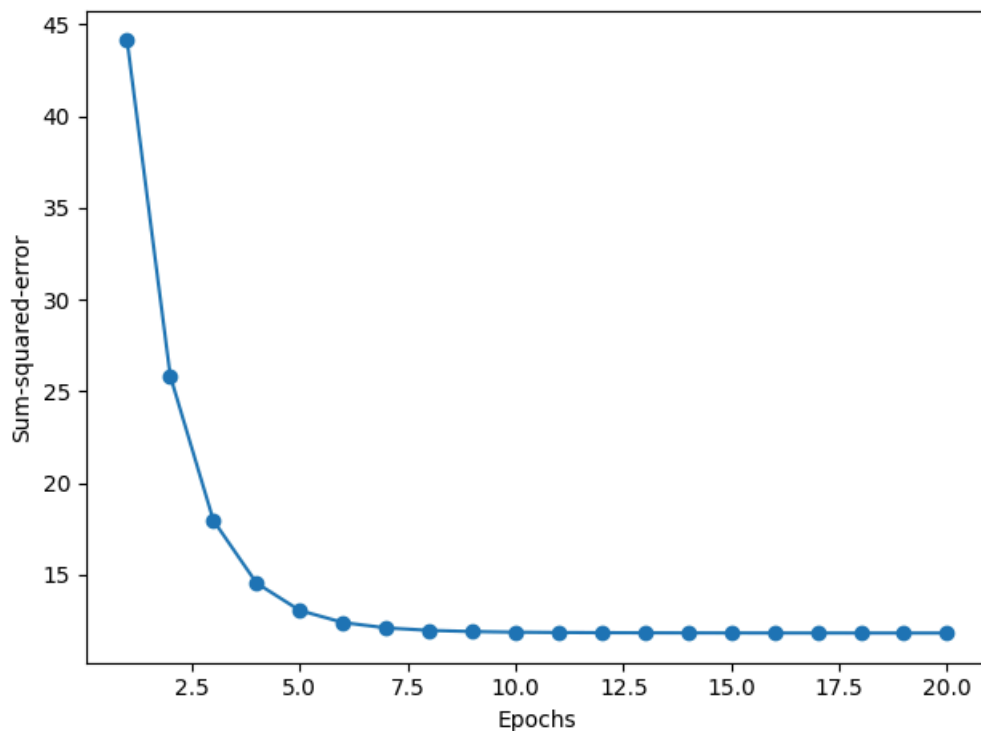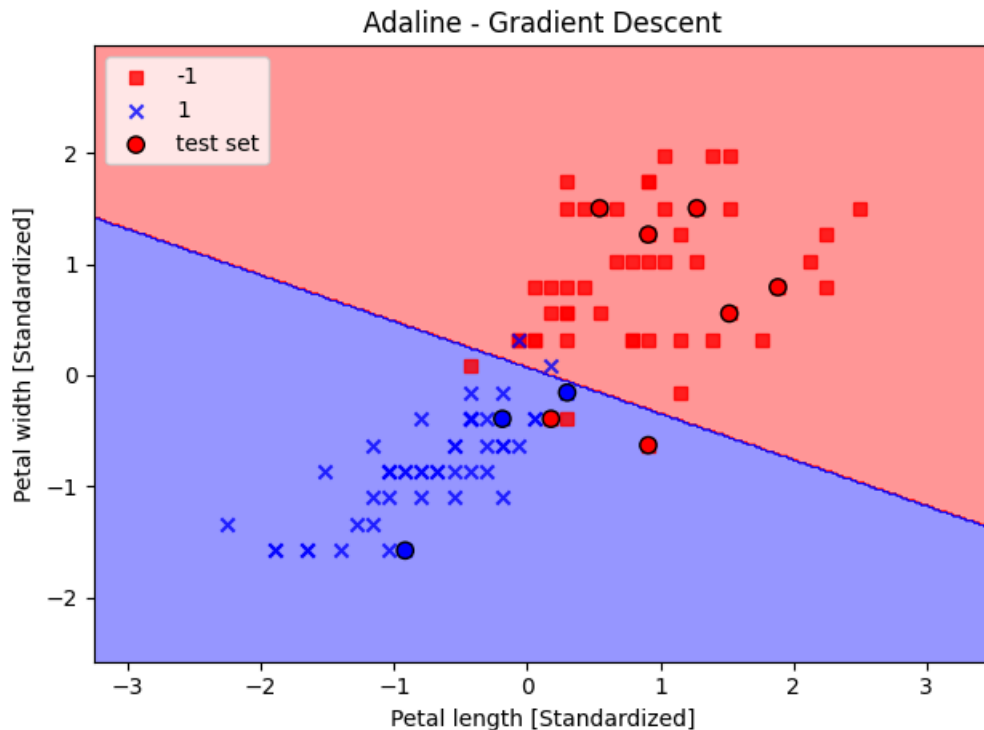
```
plt.title('Adaline - Gradient Descent')
plt.xlabel('Petal length [Standardized]')
plt.ylabel('Petal width [Standardized]')
plt.legend(loc='upper left')
plt.tight_layout()
plt.savefig('./output/fig-adaline-gd-boundary.png', dpi=300)
plt.show()
```



```
Misclassified samples: 2
Accuracy: 0.80
```


Implementing Adaline with SGD

Running the gradient descent can be computationally costly when the number of examples N in a training dataset is large since we need to scan the entire dataset every time to take one descent step. The stochastic gradient descent (SGD) update the weights incrementally for each minibatch of size M, $M \ll N$. SGD usually reaches convergence much faster because of the more frequent weight updates. Since each gradient

is calculated based on few training examples, the point taken at each step may "wander" randomly and the cost value may not always decrease. However, this may be considered as an advantage in that it can escape shallow local minima when the cost function is not convex. To prevent SGD from wandering around the optimal point, we often replace the constant learning rate η by an adaptive learning rate that decreases over time. For example, we can let

$$\eta = \frac{a}{t+b},$$

where t is the iteration number and a and b are constants. Furthermore, to hold the assumption that each minibatch consists of "randomly sampled" points from the same data generation distribution when we regard the cost function as an expectation, it is important to feed SGD with data in a random order, which is why we shuffle the training set for every epoch.

Let's implement the Adaline with SGD. For simplicity, we use a constant learning rate and set $M = 1$:

```
In [15]: class AdalineSGD(object):
    """"ADAptive LInear NEuron classifier.

    Parameters
    ------------
    eta : float
        Learning rate (between 0.0 and 1.0)
    n_iter : int
        Passes over the training dataset.

    Attributes
    -----------
    w_ : 1d-array
        Weights after fitting.
    errors_ : list
        Number of misclassifications in every epoch.
    shuffle : bool (default: True)
        Shuffles training data every epoch if True to prevent cycles.
    random_state : int
        Set random state for shuffling and initializing the weights.

    """
    def __init__(self, eta=0.01, n_iter=50, shuffle=True, random_state=1):
        self.eta = eta
        self.n_iter = n_iter
        self.w_initialized = False
        self.shuffle = shuffle
        if random_state : seed(random_state)

    def fit(self, X, y):
        """ Fit training data.

        Parameters
        ----------
        X : array-like; 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 or labels.

        Returns
        -------
        self : object

        """
        self._initialize_weights(X.shape[1])
        self.cost_ = []
        for i in range(self.n_iter):
            if self.shuffle:
                X, y = self._shuffle(X, y)
            cost = []
            for xi, yi in zip(X, y):
                cost.append(self._update_weights(xi, yi))
            avg_cost = sum(cost) / len(y)
            self.cost_.append(avg_cost)
        return self
```

```python
    def _shuffle(self, X, y):
        """Shuffle training data"""
        r = np.random.permutation(len(y))
        return X[r], y[r]

    def _initialize_weights(self, m):
        """Randomly initialize weights"""
        self.w_ = np.random.normal(loc=0.0, scale=0.01, size=1 + m)
        self.w_initialized = True

    def _update_weights(self, xi, yi):
        """Apply Adaline learning rule to update the weights"""
        output = self.activation(xi)

        # Cost function
        error = (yi - output)
        cost = 0.5 * error**2

        # Update rule
        self.w_[1:] += self.eta * xi.dot(error)
        self.w_[0] += self.eta * error

        return cost

    def net_input(self, X):
        """Calculate net input"""
        return np.dot(X, self.w_[1:]) + self.w_[0]

    def activation(self, X):
        """Compute linear activation"""
        return self.net_input(X)

    def predict(self, X):
        """Return class label after unit step"""
        return np.where(self.activation(X) >= 0.0, 1, -1)

    def partial_fit(self, X, y):
        """Fit training data without reinitializing the weights"""
        if not self.w_initialized:
            self._initialize_weights(X.shape[1])
        if y.ravel().shape[0] > 1:
            for xi, yi in zip(X, y):
                self._update_weights(xi, yi)
        else:
            self._update_weights(X, y)
        return self
```

We pass `random_state` to `np.random.seed` so it will be used for shuffling and initializing the weights. If we modify the `activation()` method so that it is identical to the `predict()` method, then this class degenerates into the Perceptron with shuffling.

NOTE:

Although not shown in our implementation, setting a larger minibatch size $M > 1$ is advantages on modern CPU architecture as we can replace the for-loop over the training samples by **vectorized** operations, which is usually improve the computational efficiency. Vectorization means that an elemental arithmetic operation is automatically applied to all elements in an array. By formulating our arithmetic operations as a sequence of instructions on an array rather than performing a set of operations for each element one at a time, we can make better use of our modern CPU architectures with Single Instruction, Multiple Data (SIMD) support. Furthermore, many scientific libraries like NumPy use highly optimized linear algebra libraries, such as Basic Linear Algebra Subprograms (BLAS) and Linear Algebra Package (LAPACK) that implement vectorized operations in C or Fortran.

Let's see how Adaline performs with SGD:

```python
In [16]: adas = AdalineSGD(n_iter=20, eta=0.01, random_state=1)
         adas.fit(X_train_std, y_train)

         # Cost values
```

```python
plt.plot(range(1, len(adas.cost_) + 1), adas.cost_,
         marker='o', label='SGD')
plt.plot(range(1, len(ada.cost_) + 1), np.array(ada.cost_) / len(y_train),
         marker='x', linestyle='--', label='GD')
plt.xlabel('Epochs')
plt.ylabel('Sum-squared-error')
plt.legend(loc='upper right')

plt.tight_layout()
plt.savefig('./output/fig-adaline-sgd-cost.png', dpi=300)
plt.show()

# Testing accuracy
y_pred = adas.predict(X_test_std)
print('Misclassified samples: %d' % (y_test != y_pred).sum())
print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))

# Plot decision boundary
plot_decision_regions(X_combined_std, y_combined,
                      classifier=adas, test_idx=range(len(y_train),
                                                      len(y_train) + len(y_test)))
plt.title('Adaline - Stochastic Gradient Descent')
plt.xlabel('Petal length [Standardized]')
plt.ylabel('Petal width [Standardized]')
plt.legend(loc='upper left')
plt.tight_layout()
plt.savefig('./output/fig-adaline-sgd-boundary.png', dpi=300)
plt.show()
```
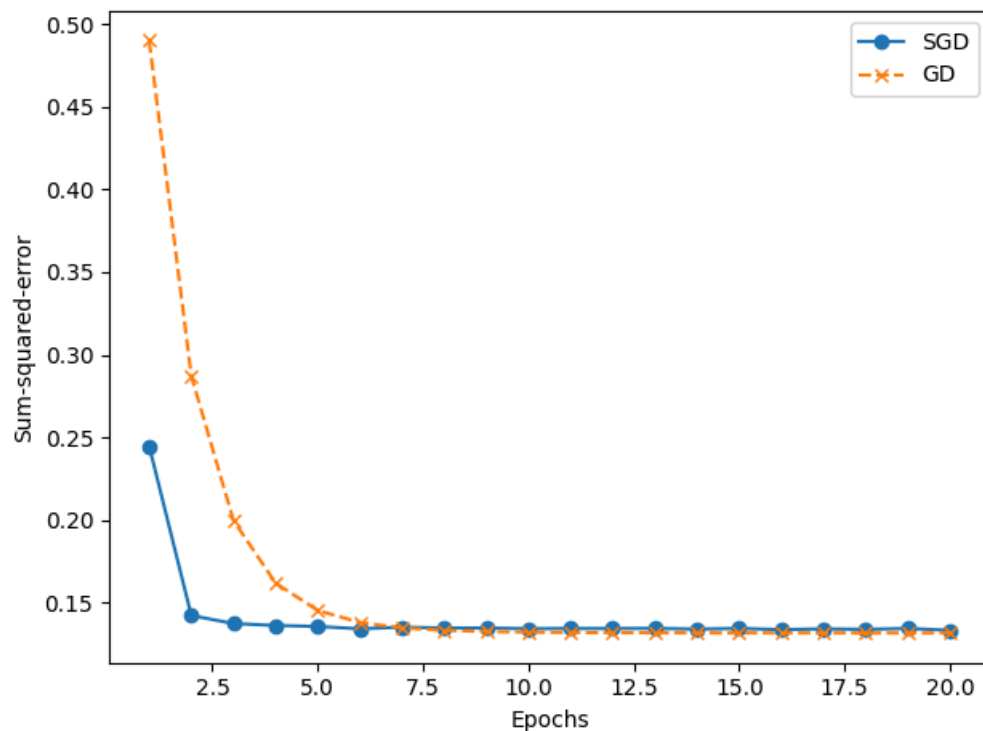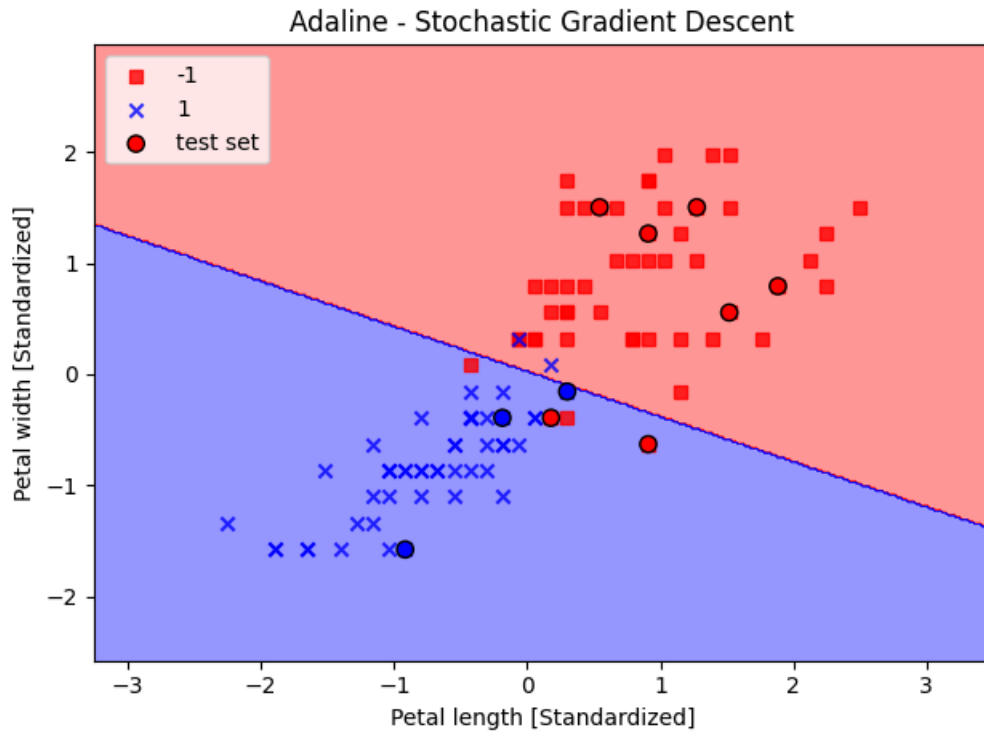


```
Misclassified samples: 2
Accuracy: 0.80
```

As we can see, the cost value goes down pretty quickly, and is only sightly worse than the (normalized) cost value of the batch gradient descent after 7 epochs.

Another advantage of stochastic gradient descent is that we can use it for **online learning**. In online learning, a model is trained on-the-fly as new training data arrives. This is especially useful if we are accumulating large amounts of data over time. For example, customer data in typical web applications. Using online learning, the system can immediately adapt to changes without training from the scratch. Furthermore, if storage space is an issue, we can discard the training data after updating the model. In our implementation, we provide the `partial_fit()` method for online learning.

Assignment

Implement the Adaline with SGD which can set different batch_size (M) as parameter. Then, use the Iris dataset to fit your model with 3 different M (including $M = 1$) and fixed learning rate η and print out the accuracy of each model. Last, plot the cost against the number of epochs using different M in one figure.

Requirements:

- Submit to **eeclass** with your code file `Lab04-1_{student_id}.ipynb` and image file `Lab04-1_{student_id}.png` (e.g. `Lab04-1_110069999.ipynb`).
- **The code file should only contain the Assignment part.**
- You can take the model we taught in lab as reference.
- To simplfy your work, you can ignore part of data which is not divisible by M.
- Deadline: **2025-12-19 (Fri) 23:59**.

Your code file should contain:

1. Split training and testing data (test_size = 20% of the whole dataset)
2. Handcrafted Adaline classifier with M as parameter.
3. Fit model with 3 different M and fixed η. (including M=1)
4. Print the accuracy of each model.
5. Plot the cost against the number of epochs using different M in one figure.

Your image file should contain:

1. Figure of the cost against the number of epochs using different M.

In [17]:
```python
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from IPython.display import display

df = pd.read_csv('https://archive.ics.uci.edu/ml/'
        'machine-learning-databases/iris/iris.data', header=None)
df.columns = ['Sepal length', 'Sepal width', 'Petal length', 'Petal width', 'Class label']
display(df.head())

X = df[['Petal length', 'Petal width']].values
y = pd.factorize(df['Class label'])[0]

# discard exmaples in the first class
X = X[50:150]
y = np.where(y[50:150] == 2, -1, y[50:150])

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=1)

sc = StandardScaler()
sc.fit(X_train)
X_train_std = sc.transform(X_train)
X_test_std = sc.transform(X_test)

print('# Training data points: %d' % X_train.shape[0])
print('# Testing data points: %d' % X_test.shape[0])
print('Class labels: %s' % np.unique(y))
```

	Sepal length	Sepal width	Petal length	Petal width	Class label
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

```
# Training data points: 80
# Testing data points: 20
Class labels: [-1  1]
```