Lecture 6: Training II

Stochastic gradient descent

Problems with batch gradient descent

- Uses the entire training set to compute gradients at every step (slow when the training set is large).
- Full training set needs to be held in memory.

Properties of stochastic gradient descent

- Uses a (random) single instance from the training set to compute gradients at each iteration (fast since very little data considered for each iteration).
- Only one instance of training data then needs to be held in memory.
- Less regular than batch gradient descent.
  - Helps to escape local minimia.
  - Ends up close to a minimum but continues to explore vacinity around minimum ("bounces" around).

Simulated annealing

To mitigate issue of bouncing around minimum, can reduce learning rate as algorithm proceeds.

Called *simulated annealing* by analogy with annealing in metallurgy.

Learning schedule defines how learning rate chances over time.

- If learning rate reduces too quickly, may get stuck on local minimum or end up frozen half-way to minimum.
- If learning rate reduces too slowly, may jump around minimum for long time.

Example learning schedule

Set learning rate α at iteration t by

$$\alpha(t) = \frac{t_0}{t + t_1},$$

where t_0 and t_1 are parameters.

Stochastic gradient descent example

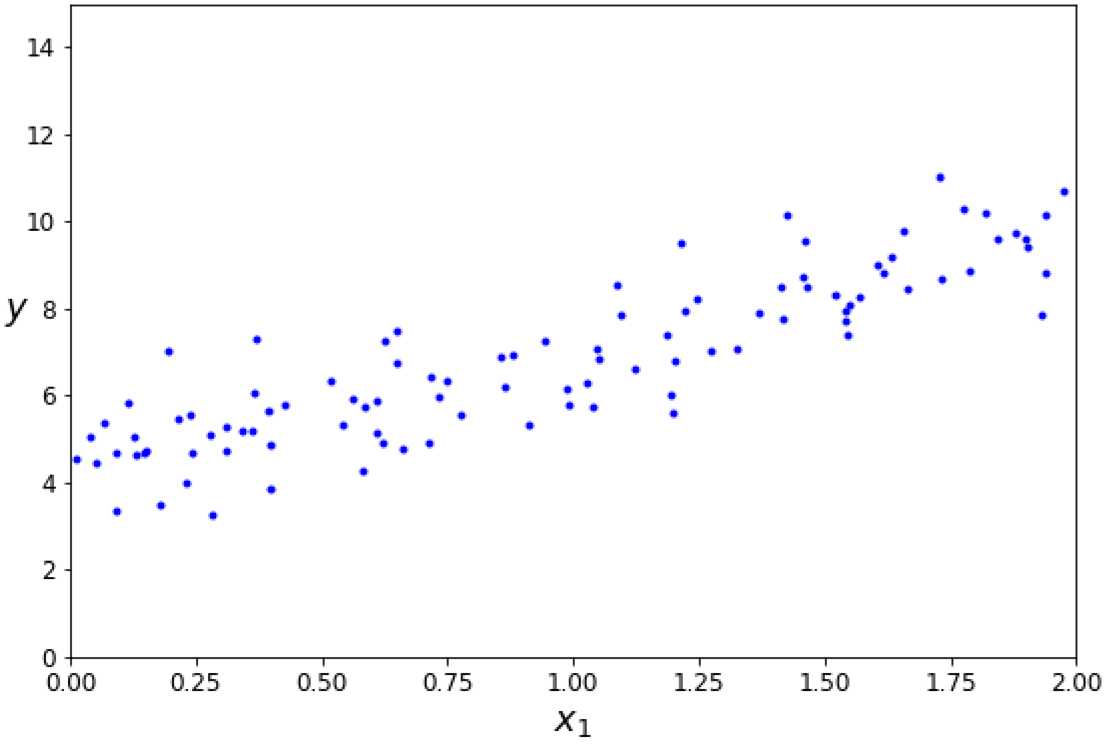
In [2]:

```
# Common imports
import os
import numpy as np
np.random.seed(42) # To make this notebook's output stable across runs

# To plot pretty figures
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt
plt.rcParams['axes.labelsize'] = 14
plt.rcParams['xtick.labelsize'] = 12
plt.rcParams['ytick.labelsize'] = 12
```

Set up training data (repeating example from previous lecture)

In [3]:
```
m = 100
X = 2 * np.random.rand(m, 1)
y = 4 + 3 * X + np.random.randn(m, 1)
plt.figure(figsize=(9,6))
plt.plot(X, y, "b.")
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$y$", rotation=0, fontsize=18)
plt.axis([0, 2, 0, 15]);
```



Add bias terms

In [4]:
```
X_b = np.c_[np.ones((m, 1)), X]          # add x0 = 1 to each instance
X_new = np.array([[0], [2]])
X_new_b = np.c_[np.ones((2, 1)), X_new] # add x0 = 1 to each instance
```

Solve by SGD with learning schedule

In [5]:

```
theta_path_sgd = []
m = len(X_b)
np.random.seed(42)

n_epochs = 50
t0, t1 = 5, 50  # learning schedule hyperparameters

def learning_schedule(t):
    return t0 / (t + t1)

theta = np.random.randn(2,1)  # random initialization
```

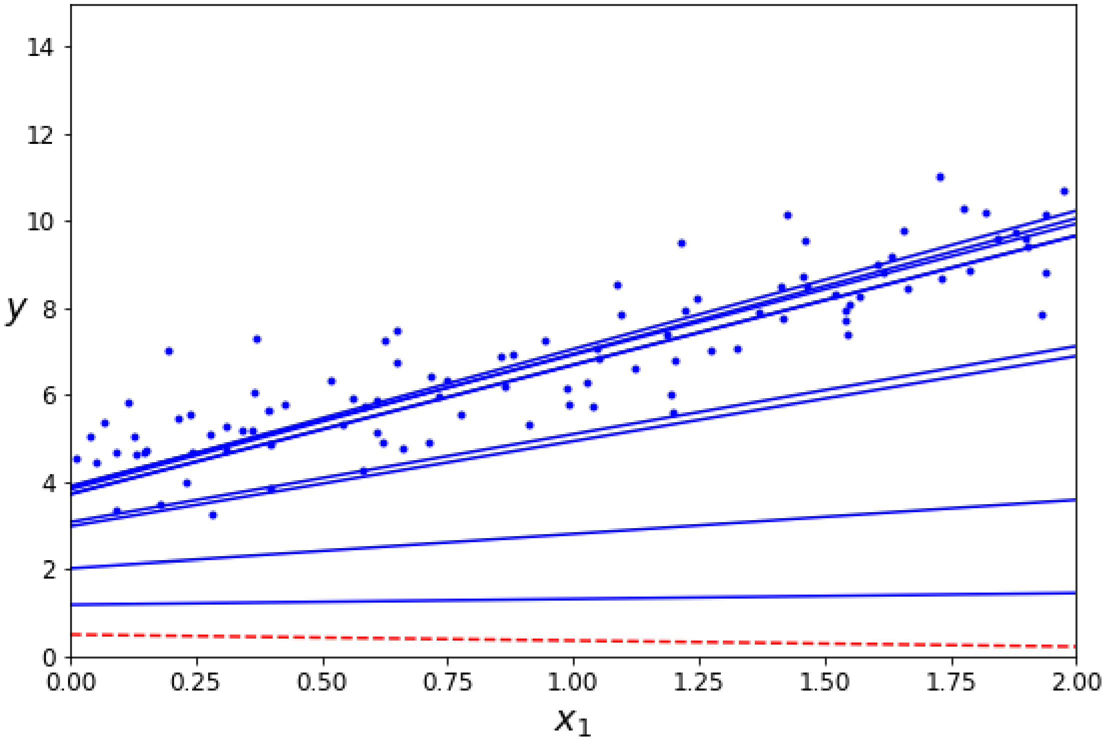
In [6]:

```
plt.figure(figsize=(9,6))
for epoch in range(n_epochs):
    for i in range(m):

        # Plot current model
        if epoch == 0 and i < 10:
            y_predict = X_new_b.dot(theta)
            style = "b-" if i > 0 else "r--"
            plt.plot(X_new, y_predict, style)

        # SGD update
        random_index = np.random.randint(m)
        xi = X_b[random_index:random_index+1]
        yi = y[random_index:random_index+1]
        gradients = 2 * xi.T.dot(xi.dot(theta) - yi)
        alpha = learning_schedule(epoch * m + i)
        theta = theta - alpha * gradients
        theta_path_sgd.append(theta)

plt.plot(X, y, "b.")
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$y$", rotation=0, fontsize=18)
plt.axis([0, 2, 0, 15]);
```



14
12
10
8
6
4
2
0
y
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
x_1

In [7]:
```
theta
```

Out[7]:
```
array([[4.21076011],
       [2.74856079]])
```

```
In [7]: theta
```

```
Out[7]: array([[4.21076011],
               [2.74856079]])
```

Use only 50 passes over the data, compared to 1000 for batch gradient descent.

Exercise: Solve using Scikit-Learn (without learning schedule)

Solve the above problem using Scikit-Learn, considering a learning rate of 0.1. Display the intercept and slope of the fitted line.

Exercise: Solve using Scikit-Learn (without learning schedule)

Solve the above problem using Scikit-Learn, considering a learning rate of 0.1. Display the intercept and slope of the fitted line.

In [8]:

```
from sklearn.linear_model import SGDRegressor
sgd_reg = SGDRegressor(max_iter=50, penalty=None, eta0=0.1, random_state=42)
sgd_reg.fit(X, y.ravel());
sgd_reg.intercept_, sgd_reg.coef_
```

Out[8]:

```
(array([4.16782089]), array([2.72603052]))
```

Mini-batch gradient descent

Use *mini-batches* of small random sets of instances of training data.

Trades off properties of batch GD and stochastic GD.

Can get a performance boost over SGD by exploiting hardware optimisation for matrix operations, particularly for GPUs.

Shuffling training data

First step is to randomly shuffle or reorder data-set since do not want to be sensitive to ordering of data (want mini-batch considered to be representative).

Exercise: implement a mini-batch gradient descent algorithm to solve previous problem.

Hints:

- May want to start with stochastic GD implementation and adapt it.
- The numpy function `np.random.permutation` (https://docs.scipy.org/doc/numpy/reference/generated/numpy.random.permutation.htm may be useful.

In [9]:
```
theta_path_mgd = []

n_iterations = 50
minibatch_size = 20

np.random.seed(42)
theta = np.random.randn(2,1)  # random initialization

t0, t1 = 5, 50
def learning_schedule(t):
    return t0 / (t + t1)

t = 0
for epoch in range(n_iterations):
    shuffled_indices = np.random.permutation(m)
    X_b_shuffled = X_b[shuffled_indices]
    y_shuffled = y[shuffled_indices]
    for i in range(0, m, minibatch_size):
        t += 1
        xi = X_b_shuffled[i:i+minibatch_size]
        yi = y_shuffled[i:i+minibatch_size]
        gradients = 2/minibatch_size * xi.T.dot(xi.dot(theta) - yi)
        eta = learning_schedule(t)
        theta = theta - eta * gradients
        theta_path_mgd.append(theta)

theta
```

Out[9]:
```
array([[4.18223159],
       [2.79659366]])
```

Comparing gradient descent algorithms

Repeat batch gradient descent from previous lecture

In [10]:

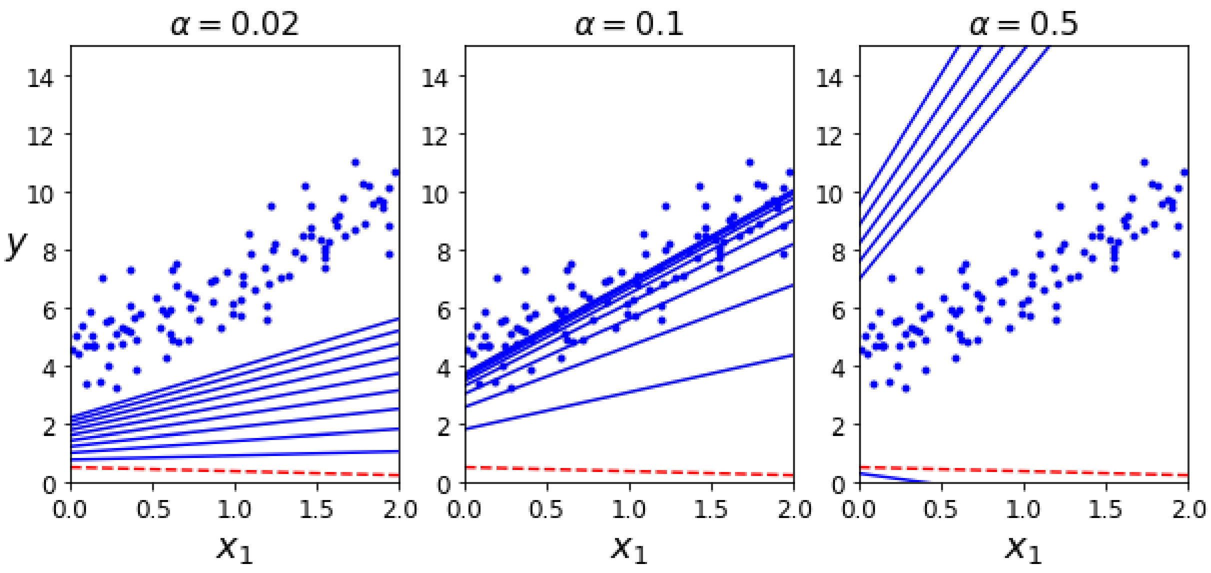
```
theta_path_bgd = []

def plot_gradient_descent(theta, alpha, theta_path=None):
    m = len(X_b)
    plt.plot(X, y, "b.")
    n_iterations = 1000
    for iteration in range(n_iterations):
        if iteration < 10:
            y_predict = X_new_b.dot(theta)
            style = "b-" if iteration > 0 else "r--"
            plt.plot(X_new, y_predict, style)
        gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)
        theta = theta - alpha * gradients
        if theta_path is not None:
            theta_path.append(theta)
    plt.xlabel("$x_1$", fontsize=18)
    plt.axis([0, 2, 0, 15])
    plt.title(r"$\alpha = {}$".format(alpha), fontsize=16)
```

In [11]:

```
np.random.seed(42)
theta = np.random.randn(2,1)  # random initialization

plt.figure(figsize=(10,4))
plt.subplot(131); plot_gradient_descent(theta, alpha=0.02)
plt.ylabel("$y$", rotation=0, fontsize=18)
plt.subplot(132); plot_gradient_descent(theta, alpha=0.1, theta_path=theta_path_bg
d)
plt.subplot(133); plot_gradient_descent(theta, alpha=0.5)
```



Convert lists to numpy arrays

In [12]:

```
theta_path_bgd = np.array(theta_path_bgd)
theta_path_sgd = np.array(theta_path_sgd)
theta_path_mgd = np.array(theta_path_mgd)
```

Algorithm trajectories

In [13]:

```
plt.figure(figsize=(10,5))
plt.plot(theta_path_sgd[:, 0], theta_path_sgd[:, 1], "r-s", linewidth=1, label="St
ochastic")
plt.plot(theta_path_mgd[:, 0], theta_path_mgd[:, 1], "g-+", linewidth=2, label="Mi
ni-batch")
plt.plot(theta_path_bgd[:, 0], theta_path_bgd[:, 1], "b-o", linewidth=3, label="Ba
tch")
plt.legend(loc="upper left", fontsize=16)
plt.xlabel(r"$\theta_0$", fontsize=20)
plt.ylabel(r"$\theta_1$   ", fontsize=20, rotation=0)
plt.axis([2.5, 4.5, 2.3, 3.9]);
```