Lab 2 Exercises for COMP 432 Machine Learning

In this lab you'll translate mathematics from lecture into practical Numpy code. Specifically, you'll implement *linear least squares regression* and *logistic regression* "from scratch" and compare the results of your own implementations to those of *scikit-learn*, a popular machine learning package.

Warning. Many of the code cells in this notebook re-use the variable names like `X` or `y`, but assign them different data. If you run cells out of order, you may get unexpected results or errors, so be careful when switching between exercises.

Run the code cell below to import the required packages.

In [258…

```python
import numpy as np
import matplotlib.pyplot as plt
import sklearn
import sklearn.linear_model
```

Lab2 requires a good understanding of Numpy and Matplotlib. Please complete Lab1 before attempting Lab2.

---

1. Plotting a 2D function and its gradient

Exercises 1.1–1.4 ask you to plot a function and its gradient, then optimize it with gradient descent.

Exercise 1.1 — Evaluate a function on a 2D grid

The Python function below takes another function, *func*, as an argument, and evaluates it on a 2D grid.

In [259…

```python
def eval_on_grid_unvectorized(func, extent, numsteps):
    """
    Evaluates func(x1, x2) for each combination in a 2D grid.
      func: callable - function to evaluate for each grid element
      extent: tuple - grid extent as (x1min, x1max, x2min, x2max)
      numsteps: int - number of grid steps (same for each dimension)
    """
    x1min, x1max, x2min, x2max = extent
    x1 = np.empty((numsteps, numsteps))
    x2 = np.empty((numsteps, numsteps))
    y  = np.empty((numsteps, numsteps))
    for i in range(numsteps):
        for j in range(numsteps):
            x1[i,j] = x1min + j*(x1max-x1min)/(numsteps-1)
            x2[i,j] = x2min + i*(x2max-x2min)/(numsteps-1)
            y[i,j] = func(x1[i,j], x2[i,j])
    return x1, x2, y
```

Run the code cell below to see an example of its output.

In [260…

```python
x1, x2, y = eval_on_grid_unvectorized(lambda x1, x2: x1 + x2, (-1, 1, 0, 2), 3)
print("x1:"); print(x1)
print("x2:"); print(x2)
print("y:");  print(y)
```

```
x1:
[[-1.  0.  1.]
 [-1.  0.  1.]
 [-1.  0.  1.]]
x2:
[[0. 0. 0.]
 [1. 1. 1.]
 [2. 2. 2.]]
y:
[[-1.  0.  1.]
 [ 0.  1.  2.]
 [ 1.  2.  3.]]
```

Write a vectorized version of *eval_on_grid* in the code cell below. Your code should be fully vectorized, with no for-loops. Consider using *np.meshgrid* and *np.linspace*.

In [261…

```python
def eval_on_grid_vectorized(func, extent, numsteps):
    # Your code here. Aim for 4-6 lines.
    x = np.linspace(extent[0], extent[1], numsteps)
    y = np.linspace(extent[2], extent[3], numsteps)
    x1, x2 = np.meshgrid(x, y)
    return x1, x2, func(x1, x2),
```

Check your answer by running the code cell below.

In [262…

```python
args = (lambda x1, x2: x1 * x2, (-1, 1, -4, 4), 20)
r1 = eval_on_grid_unvectorized(*args)       # r1 = (x1, x2, y) for unvec version
r2 = eval_on_grid_vectorized(*args)         # r2 = (x1, x2, y) for vec version
for v1, v2 in zip(r1, r2):
    np.testing.assert_almost_equal(v1, v2)  # check that x1, x2, or y matches
print("Correct!")

import timeit
args = (lambda x1, x2: x1**2 + 0.5*x2, (0, 1, 0, 1), 200)
unvec_time = timeit.timeit('eval_on_grid_unvectorized(*args)', setup="from __main__ import eval_on_grid_unvecto
vec_time   = timeit.timeit('eval_on_grid_vectorized(*args)',   setup="from __main__ import eval_on_grid_vectori
print("Your vectorized code ran %.1fx faster than the original code on a 200x200 grid" % (unvec_time/vec_time))
```

```
Correct!
Your vectorized code ran 294.4x faster than the original code on a 200x200 grid
```

Exercise 1.2 — Plot a function as a heatmap

Consider the function

$$f(x_1, x_2) = (\tfrac{1}{2}x_1 + x_2 + 1)^2 + (x_2 - 1)^2$$

Write code to compute $f(x_1, x_2)$. Your code should run for x_1 and x_2 either numbers or Numpy arrays.

In [263…

```python
def f(x1, x2):
    # Your code here. Aim for 1-3 lines.
    return (0.5 * x1 + x2 +1)**2 + (x2 - 1)**2
```

Check your answer by running the code cell below.

In [264…

```python
v = f(2.5, -4.0)
assert isinstance(v, float), "Expected float args to give float result"
assert v == 28.0625, "Wrong return value for float"
v = f(np.eye(3, 4), np.arange(12).reshape(3, 4))
assert isinstance(v, np.ndarray), "Expected ndarray args to give ndarray result"
np.testing.assert_equal(v, [[3.25, 4., 10., 20.], [34., 58.25, 74., 100.], [130., 164., 213.25, 244.]])
print("Correct!")
```

```
Correct!
```

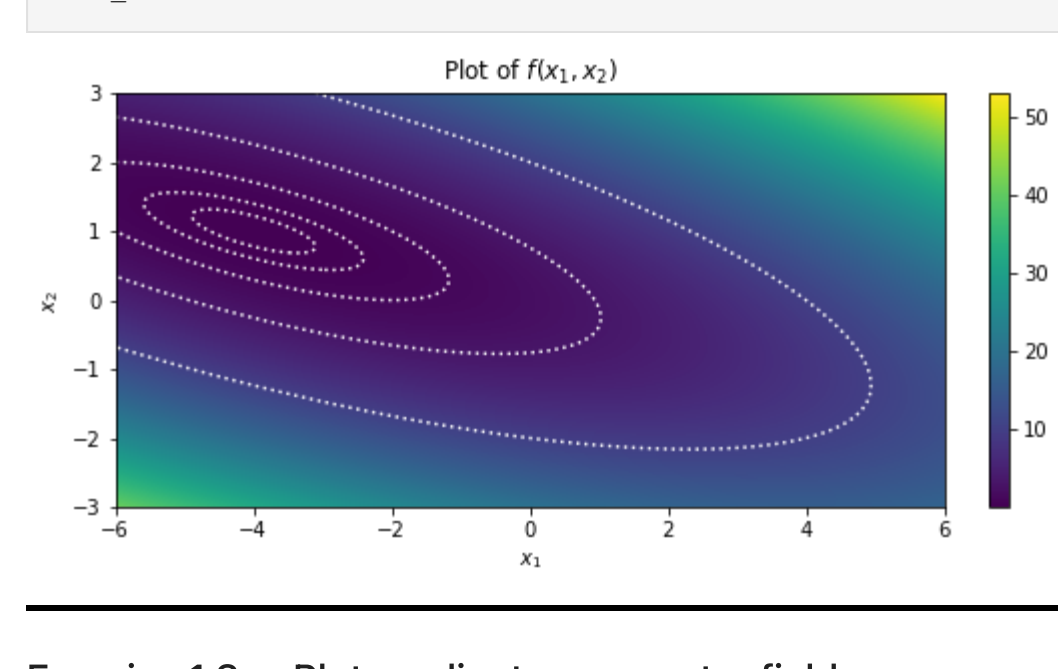
Write plotting code to visualize your $f(x_1, x_2)$ function over the interval $x_1 \in [-6, 6]$ and $x_2 \in [-3, 3]$. Your plot should look like this:

Specifically:

- Use your *eval_on_grid_vectorized* to compute all the grid positions and function values at sufficient resolution.
- Use *plt.figure* with a *figsize* designed to make the plot twice as wide as it is tall
- Use *plt.imshow* and specify *origin* and *extent* to ensure the function values are plotted at the right positions.
- Use *plt.colorbar* and specify *fraction=0.046/2* to make its height match the main figure
- Use *plt.contour* and use *np.logspace* to plot 5 contours logarithmically spaced between 0.1 and 10 inclusive.
- Configure the axis labels and title.

In [265…

```python
def plot_exercise12():
    # Your code here. Aim for 9-12 lines.
    x1, x2, y = eval_on_grid_vectorized(f, (-6, 6, -3, 3), 1000)
    plt.figure(num='$f(x_1, x_2)$', figsize=(8, 4))
    plt.imshow(y, origin='lower', extent=[-6, 6, -3, 3])
    plt.colorbar(fraction=0.0462/2)
    plt.contour(x1, x2, y, np.logspace(-1, 1, num=5), colors='w', linestyles='dotted')
    plt.ylabel('$x_2$')
    plt.xlabel('$x_1$')
    plt.title('Plot of $f(x_1, x_2)$')
plot_exercise12()
```



Exercise 1.3 — Plot gradients as a vector field

The gradient of $f(x_1, x_2)$ is a vector-valued function:

$$\nabla f(x_1, x_2) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x_1, x_2) \\ \frac{\partial f}{\partial x_2}(x_1, x_2) \end{bmatrix}$$

Write code to compute $\nabla f(x_1, x_2)$. You'll need to use basic calculus (differentiation) to figure out the correct formulas to implement, by yourself. Consider using *np.stack* to form the final array of gradients.

In [266…

```python
def f_grad(x1, x2):
    """
    Returns an ndarray 'grad' where grad[0,...] and grad[1,...] are the 1st and
    2nd gradient components (respectively) when evaluated at x1[...] and x2[...].
    In other words, if x1 and x2 have shape (...) then grad has shape (2,...).
    """
    # Your code here. Aim for 1-3 lines.
#     (0.5 * x1 + x2 +1)**2 + (x2 - 1)**2
    return np.stack([(2*(0.5 * x1 + x2 +1) * 0.5), (2*(0.5 * x1 + x2 +1) + 2*(x2 - 1))])
```

Check your answer by running the code cell below.

In [267…

```python
v = f_grad(3.5, -15.0)
assert isinstance(v, np.ndarray), "Expected float args to give ndarray result"
np.testing.assert_equal(v, [-12.25, -56.5])
v = f_grad(np.eye(3, 4), np.arange(12).reshape(3, 4))
assert isinstance(v, np.ndarray), "Expected array args to give ndarray result"
assert v.shape == (2, 3, 4), "Result was wrong shape"
np.testing.assert_equal(v, [[[ 1.5,  2. ,  3. ,  4. ], [ 5. ,  6.5,  7. ,  8. ], [ 9. , 10. , 11.5, 12. ]],
                            [[ 1. ,  4. ,  8. , 12. ], [16. , 21. , 24. , 28. ], [32. , 36. , 41. , 44. ]]])
print("Correct!")
```

```
Correct!
```

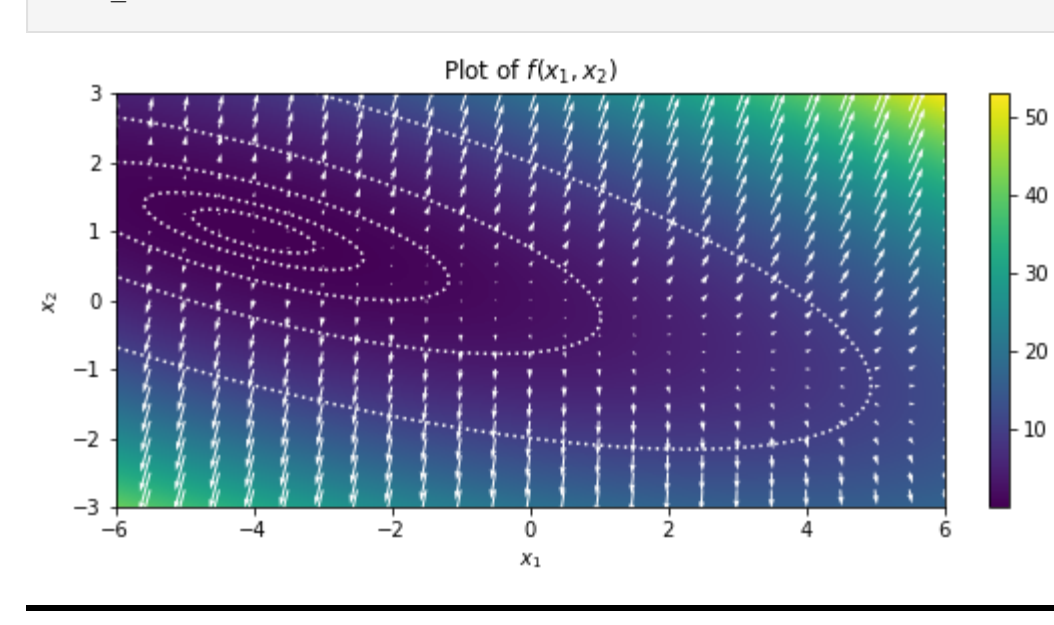
Write plotting code to overlay the gradient $\nabla f(x_1, x_2)$ over your figure from Exercise 1.2. Your plot should look like this:

Specifically:

- Use your *eval_on_grid_vectorized* to compute all the grid positions and gradient values at suitable resolution.
- Use *plt.quiver* to plot the vector field of gradients.

In [268…

```python
def plot_exercise13():
    plot_exercise12()  # Start with your previous plot

    # Your code here. Aim for 2-4 lines.
    a, b, z = eval_on_grid_vectorized(f_grad, (-6, 6, -3, 3), 25)
    plt.quiver(a, b, z[0], z[1], color='w')

plot_exercise13()
```



Exercise 1.4 — Gradient descent on a function

Gradient descent is an iterative algorithm that repeatedly takes steps in the direction opposite the gradient:

$$\mathbf{x}_{\text{new}} = \mathbf{x}_{\text{old}} - \eta \nabla f(\mathbf{x}_{\text{old}})$$

where $\mathbf{x} = (x_1, x_2)$. The step size is scaled by the *learning rate*, which is chosen to be some constant $\eta > 0$.

Write a function that runs a specific number of steps of gradient descent on the function $f(x_1, x_2)$ from Exercise 1.2. To do this, use the *f_grad* function that you wrote for Exercise 1.3.

In [269…

```python
def gradient_descent_on_f(x_init, learn_rate, num_steps):
    """
    Runs num_steps of gradient descent from point x_init using
    the given learning rate, and returns the new x coordinate.
    Here x_init is an ndarray with shape (2,).
    """
    # Your code here. Aim for 4-5 lines.
    for i in range(num_steps):
        x_init = x_init -  learn_rate * f_grad(x_init[0], x_init[1])
    return x_init
```

Check your answer by running the code cell below

In [270…

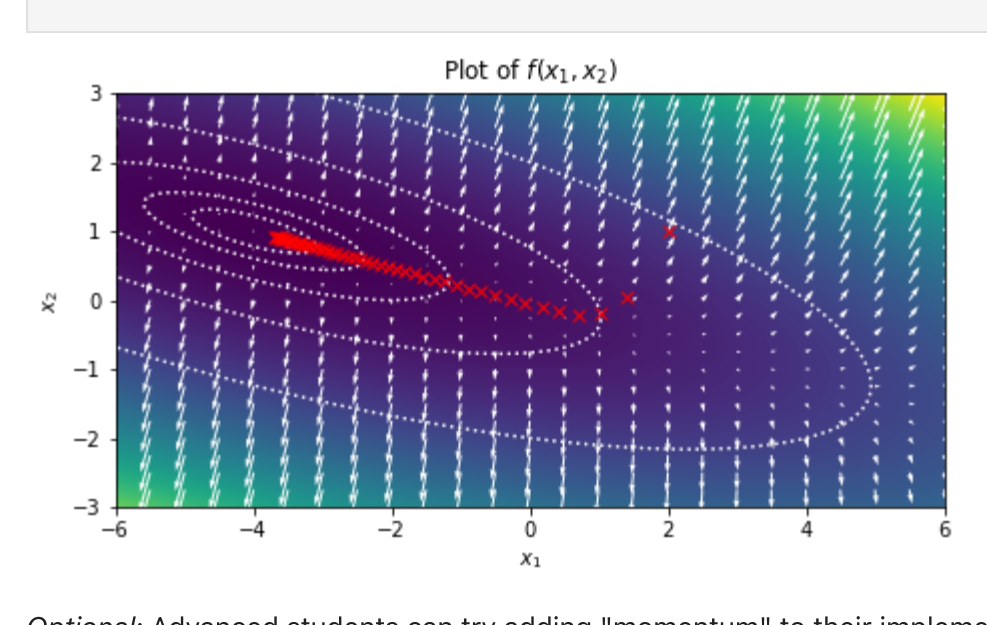
```python
x = gradient_descent_on_f(np.array([-4, 1]), 100.0, 1)
assert isinstance(x, np.ndarray), "Expected ndarray"
assert np.array_equal(x, [-4, 1]), "Gradient descent shouldn't move away from optimal value!"
x = gradient_descent_on_f(np.array([2, 0]), 0.25, 1)
assert np.array_equal(x, [1.5, -0.5]), "The first gradient step seems to be wrong!"
x = gradient_descent_on_f(x, 0.1, 3)
assert np.allclose(x, [1.1294375, -0.369625]), "The gradient seems to be wrong after a few steps!"
print("Correct!")
```

```
Correct!
```

Plot the path of gradient descent by running the code cell below. You should see a path of little red 'x' marks that converge near $(x_1^*, x_2^*) = (-4, 1)$.

In [271…

```python
plot_exercise13()  # Plot the vector field first

# Run gradient descent in chunks of 5 steps at a time, plotting the resulting 'x' after each chunk
learn_rate = 0.05
x_init = np.array([2.0, 1.0])                            # Start from initial point (-2, -1)
for num_steps in range(0, 250, 5):                        # Repeatedly run gradient descent from the initia
    x = gradient_descent_on_f(x_init, learn_rate, num_steps)  # eventually running it for 100 steps.
    plt.plot(*x, 'xr');                                  # Add a little 'x' to the plot to show how far it go
```



Optional: Advanced students can try adding "momentum" to their implementation of *gradient_descent_on_f*, and then see how it effects the path of optimization. Relevant formulas and helpful visualizations regarding momentum can be found for example in *Why Momentum Really Works*.

---

2. Linear least squares regression

Exercises 2.1–2.5 ask you to implement linear least squares regression, and to compare your results to applying the scikit-learn **LinearRegression** model.

Exercise 2.1 — Vectorized code for generating predictions from a basic linear model

Recall from Lecture 1 that a basic linear model has the form:

$$\hat{y}(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T\mathbf{w}$$

where

$$\mathbf{x} = [1 \quad x_1 \quad \dots \quad x_D]^T \qquad (1)$$
$$\mathbf{w} = [w_0 \quad w_1 \quad \dots \quad w_D]^T \qquad (2)$$

If both $\mathbf{x}$ and $\mathbf{w}$ are column vectors, the following Python function would evaluate the linear model $\hat{y}(\mathbf{x}, \mathbf{w})$ correctly:

```python
def linear_model_predict(x, w):
    """Returns a prediction from linear model y(x, w) at point x using parameters w."""
    return x.T @ w   # Return the inner product (dot product) of vectors x and w
```

However, we want a version of *linear_model_predict* that vectorizes across many $\mathbf{x}$ simultaneously. Specifically, given a matrix of inputs:

$$X = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix}$$

we want *linear_model_predict* to compute a vector of outputs:

$$\hat{\mathbf{y}} = \begin{bmatrix} \mathbf{x}_1^T\mathbf{w} \\ \vdots \\ \mathbf{x}_N^T\mathbf{w} \end{bmatrix}$$

However, if we substitute x with X we can no longer use expression `X.T @ w`; the matrix $X^T \in \mathbb{R}^{(D+1)\times N}$ isn't even the right shape to be on the left-hand side of the product. Writing vectorized code is full of annoying little problems like this.

Write a function that evaluates the linear model in vectorized fashion. Specifically, when given a matrix $X \in \mathbb{R}^{N\times(D+1)}$ as an argument, you should figure out what mathematical expression would result in the $\hat{\mathbf{y}} \in \mathbb{R}^N$ vector shown above. Hint: the solution is only a small change from `X.T @ w`.

In [272…

```python
def linear_model_predict(X, w):
    """
    Returns predictions from linear model y(X, w) at each point X[i,:] using parameters w.
    Given X with shape (N,D+1), w must have shape (D+1,) and the result will have shape (N,).
    """
    # Your code here. Aim for 1 line.
    return X @ w
```

Check your answer by running the code cell below.

In [273…

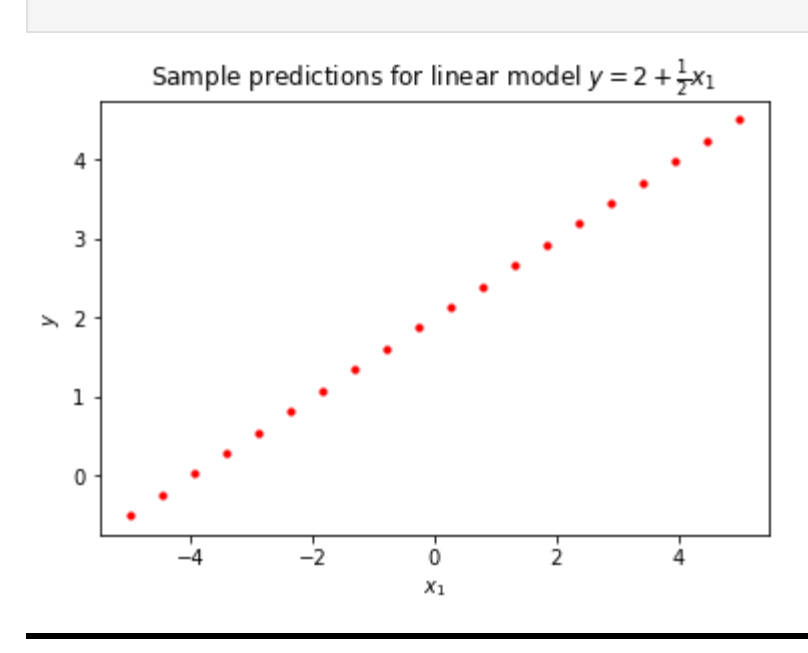
```python
w = np.array([2, 0.5])                               # Parameters corresponding to the 1D line y = 2 + 0.5*x1
X = np.array([[1., -3.], [1.,  3.], [1.,  5.]])      # Evaluate at x1 = -3, 2, 5
y = linear_model_predict(X, w)                       # Predict y for all X using w
assert isinstance(y, np.ndarray), "Expected an ndarray!"
assert np.array_equal(y, [0.5, 3.5, 4.5]), "Wrong predictions!\n%s" % y
try:
    y = linear_model_predict(X, w.reshape(-1, 1))
except ValueError:
    raise AssertionError("Your answer works when 'w' is 1-dimensional, but not when it is a column vector. Try
w = np.array([1, 0.5, 0.25])                         # Parameters corresponding to the 2D plane y = 1 + 0.5*x1 + (
X = np.array([[1., -3., 1.], [1.,  3., 0.], [1.,  5., -2.]])    # Evaluate at different (x1, x2) points
y = linear_model_predict(X, w)                       # Predict y for all X using w
assert np.array_equal(y, [-0.25, 2.5, 3.0]), "Wrong predictions for 2-dimensional feature space!\n%s" % y
print("Correct!")
```

```
Correct!
```

Plot several predictions at once by running the code cell below.

In [274…

```python
w = np.array([2, 0.5])            # Parameters corresponding to the 1D line y = 2 + 0.5*x1
x0 = np.ones(20)                  # A column of 1s so that the bias term w[0] gets added
x1 = np.linspace(-5, 5, 20)       # A column of x values ranging from [-5, 5]
X = np.column_stack([x0, x1])     # A 20x2 matrix where X[i,:] is the ith x vector
y = linear_model_predict(X, w)    # Evaluate all x values
plt.scatter(x1, y, 10, 'r')
plt.xlabel("$x_1$")
plt.ylabel("$y$")
plt.title("Sample predictions for linear model $y=2 + \\frac{1}{2}x_1$");
```



Exercise 2.2 — Linear least squares regression by gradient descent

Here you'll implement a 'learning' algorithm for linear least squares regression. Recall from Lecture 1 that the least squares training objective is:

$$\ell(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y - \hat{y}(\mathbf{x}_i, \mathbf{w}))^2$$

The gradient for the above training objective is on the slide titled "Linear least squares *learning*" from Lecture 1. You'll need it.

Write a function to implement linear least squares regression by gradient descent. Use the `@` operator (matrix multiplication) in your answer.

In [275…

```python
def linear_regression_by_gradient_descent(X, y, w_init, learn_rate=0.05, num_steps=500):
    """
    Fits a linear model by gradient descent.

    If the feature matrix X has shape (N,D) the targets y should have shape (N,)
    and the initial parameters w_init should have shape (D,).

    Returns a new parameter vector w that minimizes the squared error to the targets.
    """
    # Your code here. Aim for 4-5 lines.
    for i in range(num_steps):
        grad = (X.T.dot(X)).dot(w_init) - X.T.dot(y)
        w_init = w_init - learn_rate * grad
    return w_init
```

Check your answer by running the code cell below.

In [276…

```python
X = np.array([[1, 0.0], [1, 1.0], [1, 2.0]])
y = np.array([4.0, 3.0, 2.0])
w = linear_regression_by_gradient_descent(X, y, np.array([0.0, 0.0]))
assert isinstance(w, np.ndarray), "Expected ndarray!"
assert w.shape == (2,), "Wrong shape for final parameters!\n%s" % w
assert np.allclose(w, [4, -1]), "Wrong values for final parameters!\n%s" % w
print("Correct!")
```

```
Correct!
```

Exercise 2.3 — Linear least squares regression by direct solution

As discussed in class, the optimal parameters $\mathbf{w}^*$ for linear least squares regression can be solved *directly*, rather than iteratively.

Write a function to solve linear least squares regression directly. Use Numpy's matrix inverse function **np.linalg.inv** in your answer.

In [277…

```python
def linear_regression_by_direct_solve(X, y):
    """Fits a linear model by directly solving for the optimal parameter vector w."""
    # Your code here. Aim for 1-2 lines.
    return np.linalg.inv((X.T.dot(X))).dot(X.T.dot(y))
```

In [278…

```python
w = linear_regression_by_direct_solve(X, y)
assert isinstance(w, np.ndarray), "Expected ndarray!"
assert w.shape == (2,), "Wrong shape for final parameters!\n%s" % w
assert np.allclose(w, [4, -1]), "Wrong values for final parameters!\n%s" % w
print("Correct!")
```

```
Correct!
```

Exercise 2.4 — Run linear least squares regression and plot the result

For this exercise you'll need to define Numpy arrays that correspond to the following training data:

$$X = \begin{bmatrix} 1 & -2.2 \\ 1 & -0.3 \\ 1 & 1.5 \\ 1 & 4.8 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} -1.2 \\ 1.5 \\ 4.2 \\ 5.3 \end{bmatrix}$$

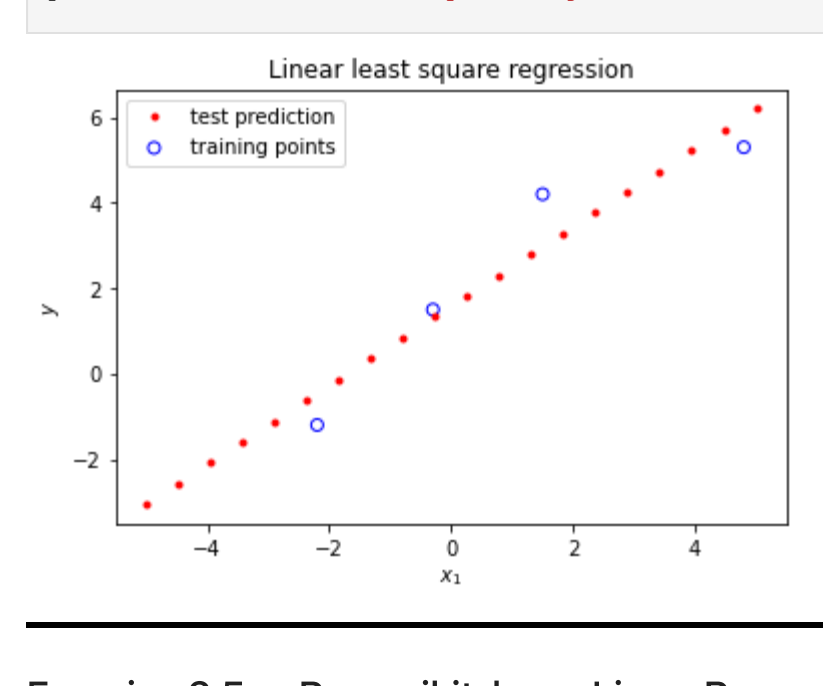
Write code to create the following plot: image

Your code should follow this sequence of steps:

1. Make ndarrays X and $\mathbf{y}$ that contain the above training set.
2. Plot the training set in blue. Use the x coordinates from the second column of X, ignoring the first column.
3. Run linear least squares regression on $(X, \mathbf{y})$ to get fitted parameters $\mathbf{w}$; use your *linear_regression_by_direct_solve* function.
4. Define a "test set" of 20 equally-spaced values of x in range $[-5, 5]$. You will need to build a new matrix X_{test} with 1 in the first column and the 20 distinct x values in the second column. See how this is done in the last code cell of Exercise 2.1.
5. Predict 20 y values corresponding to the 20 rows of X_{test} by applying a linear model with your fitted parameters $\mathbf{w}$. Do this with single call to your *linear_model_predict* function.
6. Plot the predictions on the test set.

In [279…

```python
# 1. Define the training set. Aim for 2 lines.
X = np.array([[1, -2.2], [1, -0.3], [1, 1.5], [1, 4.8]])
y = np.array([-1.2, 1.5, 4.2, 5.3])

# 2. Plot the training set. Aim for 1 line.
plt.scatter(X.T[1], y, facecolors='none', edgecolors='blue', label='training points')
# 3. Run linear least squares regression on the training set to compute 'w'. Aim for 1 line.
w = linear_regression_by_direct_solve(X, y)
# 4. Define the test set matrix of shape (20,2). Aim for 1-3 lines.
X_test = np.array([np.ones(20), np.linspace(-5, 5, num=20)]).T
# 5. Use the linear model to make predictions on the test set. Aim for 1 line.
predictions = linear_model_predict(X_test, w)
# 6. Plot the test predictions. Aim for 1 line, plus a few lines to configure the plot (axis labels etc).
plt.plot(X_test.T[1], predictions, 'or', markersize = 3, label='test prediction')
plt.xlabel('$x_1$');
plt.ylabel('$y$');
plt.legend()
plt.title('Linear least square regression');
```



Exercise 2.5 — Run scikit-learn LinearRegression

The scikit-learn package provides a **LinearRegression** object to perform linear least squares regression (also known as "ordinary" least squares).

Write code to fit a LinearRegression model using the same training matrix X that you defined as part of Exercise 2.4. There are only two steps:

1. Create the *LinearRegression* object. Use the *fit_intercept=False* option when creating the *LinearRegression* object (see documentation), since the X matrix already has a column of 1s corresponding to an intercept parameter (the 'bias' parameter).
2. Fit the *LinearRegression* object to the training matrix X and targets $\mathbf{y}$. Use the object's **fit** method.

The variable holding a reference to your *LinearRegression* object should be called `linear_model`, so that your answer can be checked.

In [286…

```python
# Your code here. Aim for 2 lines.
linear_model = sklearn.linear_model.LinearRegression(fit_intercept=False).fit(X, y)
```

Check your answer by running the code cell below.

In [284…

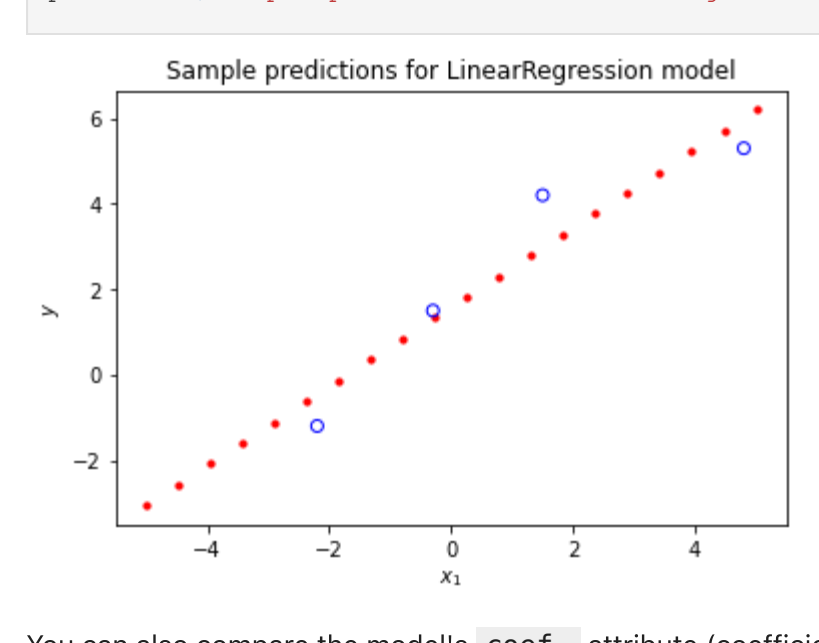
```python
assert 'linear_model' in globals(), "You didn't create a variable named 'linear_model'!"
assert isinstance(linear_model, sklearn.linear_model.LinearRegression), "Expected a LinearRegression instance!"
assert hasattr(linear_model, 'coef_'), "No model coefficients yet! You didn't fit the model to any data!"
assert linear_model.intercept_ == 0.0, "You forgot to disable fitting of the intercept!"
assert np.allclose(linear_model.coef_, [[1.57104472, 0.92521608]]), "The model parameters you learned seem inco
print("Correct!")
```

```
Correct!
```

Plot several LinearRegression model predictions at once by running the code cell below.

In [285…

```python
x0 = np.ones(20)                        # A column of 1s so that the bias term w[0] gets added
x1 = np.linspace(-5, 5, 20)             # A column of x values ranging from [-5, 5]
X_test = np.column_stack([x0, x1])      # A 20x2 matrix where X[i,:] is the ith x vector
y_test = linear_model.predict(X_test)   # Evaluate all x values
plt.scatter(x1, y_test, 10, 'r')
plt.scatter(X[:,1], y, edgecolor='b', facecolor='none')
plt.xlabel("$x_1$")
plt.ylabel("$y$")
plt.title("Sample predictions for LinearRegression model");
```



You can also compare the model's `coef_` attribute (coefficients, i.e. model parameters) to the parameter vector $\mathbf{w}$ that your own implementation gave from Exercise 2.4 (just use `print(w)` in your previous answer to see those values).

---

3. Logistic regression

Exercises 3.1–3.4 ask you to implement logistic regression, and to compare your results to applying the scikit-learn **LogisticRegression** model.

Exercise 3.1 — Vectorized code for generating predictions from a logistic model

Recall from lecture that the logistic model has the form:

$$\hat{y}(\mathbf{x}, \mathbf{w}) = \sigma(\mathbf{x}^T\mathbf{w})$$

where $\mathbf{x}$ and $\mathbf{w}$ are the same as for Exercise 2.1 and $\sigma(\cdot)$ is the logistic sigmoid function described in Lecture 1.

Write a function that evaluates the logistic model in vectorized fashion, just like you did for Exercise 2.1.

In [287…

```python
def sigmoid(z):
    """Returns the element-wise logistic sigmoid of z."""
    # Your code here. Aim for 1 line.
    return 1/(1 + np.exp(-z))

def logistic_model_predict(X, w):
    """
    Returns predictions from logistic model y(x, w) at each point X[i,:] using parameters w.
    Given X with shape (N,D+1), w must have shape (D+1,) and the result will have shape (N,).
    """
    # Your code here. Aim for 1-2 lines.
    return sigmoid(X @ w)
```

Check your answer by running the code cell below.

In [288…

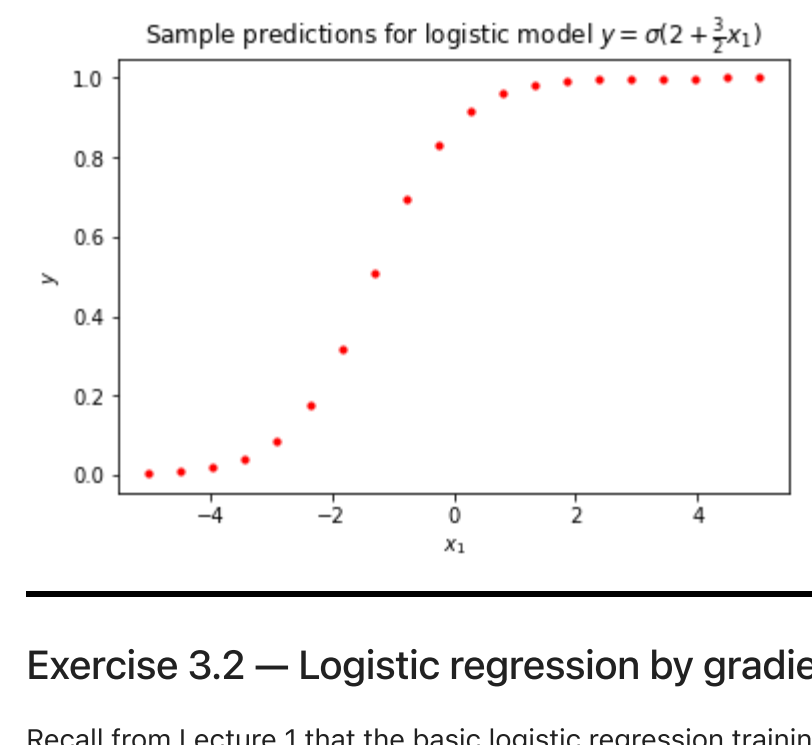
```python
y = sigmoid(np.array([-1., 0., 1.5]))
assert isinstance(y, np.ndarray), "Expected an ndarray!"
assert np.allclose(y, [0.26894142, 0.5, 0.81757448]), "Values from sigmoid() appear to be wrong!"
w = np.array([2, 1.5])                         # Parameters corresponding to logistic model y = sigmoid(2 + 1
X = np.array([[1., -2.], [1.,  0.], [1.,  2.]])   # Evaluate at x1 = -2, 0, 2
y = logistic_model_predict(X, w)               # Predict y for all X using w
assert isinstance(y, np.ndarray), "Expected an ndarray!"
assert np.allclose(y, [0.26894142, 0.88079708, 0.99330715]), "Wrong returned!\n%s" % y
try:
    y = logistic_model_predict(X, w.reshape(-1, 1))
except ValueError:
    raise AssertionError("Your answer works when 'w' is 1-dimensional, but not when it is a column vector. Try
w = np.array([1, 0.5, 0.25])                   # Parameters corresponding to the 2D plane y = 1 + 0.5*x1 + (
X = np.array([[1., -3., 1.], [1.,  3., 0.], [1.,  5., -2.]])    # Evaluate at different (x1, x2) points
y = logistic_model_predict(X, w)               # Predict y for all X using w
assert np.allclose(y, [0.4378235, 0.92414182, 0.95257413]), "Wrong predictions for 2-dimensional feature space!
print("Correct!")
```

```
Correct!
```

Plot several predictions at once by running the code cell below.

In [289…

```python
w = np.array([2, 1.5])                    # Parameters corresponding to logistic model y = sigmoid(2 + 1.5*x
x0 = np.ones(20)                          # A column of 1s so that the bias term w[0] gets added
x1 = np.linspace(-5, 5, 20)               # A column of x values ranging from [-5, 5]
X_test = np.column_stack([x0, x1])        # A 20x2 matrix where X[i,:] is the ith x vector
y_test = logistic_model_predict(X_test, w)   # Evaluate all x values
plt.scatter(x1, y_test, 10, 'r')
plt.xlabel("$x_1$")
plt.ylabel("$y$")
plt.title("Sample predictions for logistic model $y=\\sigma(2 + \\frac{3}{2}x_1)$");
```



Exercise 3.2 — Logistic regression by gradient descent

Recall from Lecture 1 that the basic logistic regression training objective (learning objective) is:

$$\ell_{\text{LR}}(\mathbf{w}) = \sum_{i=1}^{N} y_i \ln \sigma(\mathbf{w}^T\mathbf{x}_i) + (1 - y_i)\ln\big(1 - \sigma(\mathbf{w}^T\mathbf{x}_i)\big)$$

The "basic" gradient for the above training objective is on a slide titled "Maximum likelihood estimate for LR" from Lecture 1, and reproduced here:

$$\nabla\ell_{\text{LR}}(\mathbf{w}) = \sum_{i=1}^{N}(\sigma(\mathbf{w}^T\mathbf{x}_i) - y_i)\mathbf{x}_i$$

Write a function to implement logistic regression by gradient descent. Your answer to _logistic_regression*grad* should ideally be fully vectorized (no for-loops), but this may take a while to figure out. If you can't figure out the vectorization, it's OK — just compute the gradient however you can. Your answer to _logistic*regression* should use your _logistic_regression*grad* function to compute the gradient at each step.

Implementing _logistic_regression*grad* is the hardest exercise in this lab because a vectorized implementation requires using the `@` matrix multiply operator to compute all the $\mathbf{w}^T\mathbf{x}$ products, reshaping the vector of residuals into a column-vector to use Numpy's broadcasting feature, and then summing over a specific axis (over training cases $i = 1, \dots, N$).

In [298…

```python
def logistic_regression_grad(X, y, w):
    """Returns the gradient for basic logistic regression."""
    # Your code here. Aim for 1-3 lines.
    return np.dot(X.T, sigmoid(X.dot(w)) - y)

def logistic_regression(X, y, w_init, learn_rate=0.05, num_steps=500):
    """
    Fits a logistic model by gradient descent.

    If the feature matrix X has shape (N,D) the targets y should have shape (N,)
    and the initial parameters w_init should have shape (D,).

    Returns a new parameter vector w that minimizes the negative log likelihood of the targets.
    """
    # Your code here. Aim for 4-5 lines.
    for i in range(num_steps):
        grad = logistic_regression_grad(X, y, w_init)
        w_init = w_init - learn_rate * grad
    return w_init
```

Check your answer by running the code cell below.

In [299…

```python
X = np.array([[1, -1.0], [1, 1.0], [1, 2.0]])
y = np.array([0.0, 0.0, 1.0])
grad = logistic_regression_grad(X, y, np.array([0.0, 1.0]))
assert isinstance(grad, np.ndarray), "Expected ndarray from logistic_regression_grad!"
assert grad.shape == (2,), "Expected gradient to have shape (2,) but was %s" % (grad.shape,)
assert np.allclose(grad, [0.88079708, 0.22371131]), "Wrong value for gradient!"
grad = logistic_regression_grad(X, y, np.array([-1.0, 1.5]))
assert np.allclose(grad, [0.57911459, 0.30819531]), "Wrong value for gradient!"
w = logistic_regression(X, y, np.array([1.0, 0.0]))
assert isinstance(w, np.ndarray), "Expected ndarray from logistic_regression!"
assert w.shape == (2,), "Expected parameter vector w to have shape (2,) but was %s" % (w.shape,)
assert np.allclose(w, [-4.14100532, 2.95489589]), "Parameters found by gradient descent seem wrong!"
print("Correct!")
```

```
Correct!
```

Exercise 3.3 — Run logistic regression on data and plot the result

For this exercise you'll need to define Numpy arrays that correspond to the following training data:

$$X = \begin{bmatrix} 1 & -4.1 \\ 1 & -2.8 \\ 1 & -0.7 \\ 1 & 3.5 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

Write code to create the following plot: image

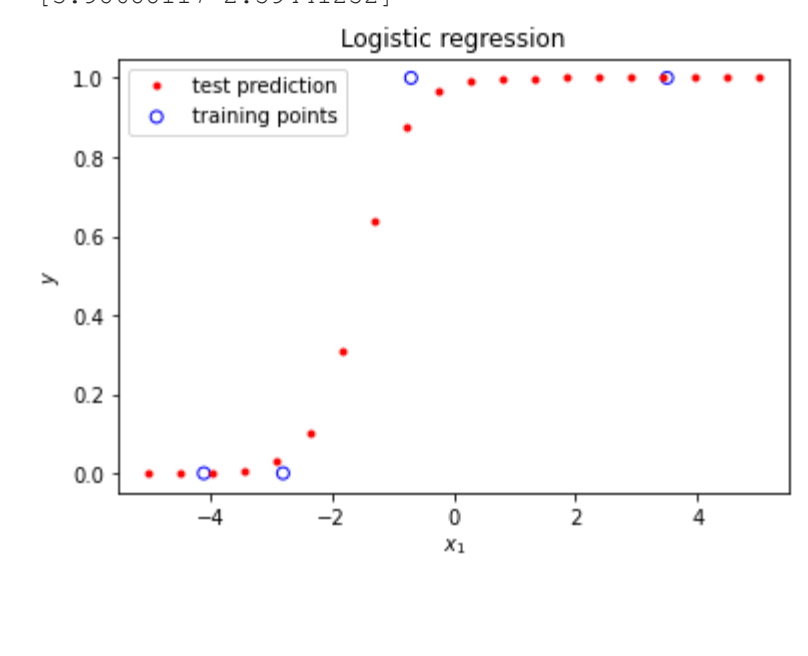
Your code should follow this sequence of steps, which are the same as for Exercise 2.4:

1. Make ndarrays X and $\mathbf{y}$ that contain the above training set.
2. Plot the training set in blue. Use the x coordinates from the second column of X, ignoring the first column.
3. Run logistic regression on $(X, \mathbf{y})$ to get fitted parameters $\mathbf{w}$; use your *logistic_regression* function, starting from $\mathbf{w}_{\text{init}} = [0.0, 1.0]^T$
4. Define a "test set" of 20 equally-spaced values of x in range $[-5, 5]$. You will need to build a new matrix X_{test} with 1 in the first column and the 20 distinct x values in the second column.
5. Predict 20 y values corresponding to the 20 rows of X_{test} by applying a logistic model with your fitted parameters $\mathbf{w}$. Do this with single call to your *logistic_model_predict* function.
6. Plot the predictions on the test set.

In [333…

```python
# 1. Define the training set. Aim for 2 lines.
X=np.array([[1, -4.1], [1, -2.8], [1, -0.7], [1, 3.5]])
y = [0, 0, 1, 1]

# 2. Plot the training set. Aim for 1 line.
plt.scatter(X.T[1], y, facecolors='none', edgecolors='blue', label='training points')

# 3. Run logistic regression on the training set to get 'w'. Aim for 1-2 lines.
w = logistic_regression(X, y, np.array([0.0, 1.0]).T)
print(w)
# 4. Define the test set matrix of shape (20,2). Aim for 1-3 lines.
X_test = np.array([np.ones(20), np.linspace(-5, 5, num=20)]).T

# 5. Use the linear model to make predictions on the test set. Aim for 1 line.
predictions = logistic_model_predict(X_test, w)

# 6. Plot the test predictions. Aim for 1 line, plus a few lines to configure the plot (axis labels etc).
plt.plot(X_test.T[1], predictions, 'or', markersize = 3, label='test prediction')
plt.xlabel('$x_1$');
plt.ylabel('$y$');
plt.legend()
plt.title('Logistic regression');
```

```
[3.98688117 2.59441252]
```



Exercise 3.4 — Run scikit-learn LogisticRegression

The scikit-learn package provides a **LogisticRegression** object to perform logistic regression.

Write code to fit a LogisticRegression model using the same training matrix X that you defined as part of Exercise 3.3. There are only two steps:

1. Create the *LogisticRegression* object. Do not fit an "intercept" and do not include any regularization penalty (see documentation).
2. Fit the *LogisticRegression* object to the training matrix X and targets $\mathbf{y}$. Use the object's **fit** method.

The variable holding a reference to your *LogisticRegression* object should be called `logistic_model`, so that your answer can be checked.

A tweet regarding the fact that scikit-learn's LogisticRegression object applies regularization (a weight penalty) "by default":
image

In [334…

```
# Your code here. Aim for 2 lines.
logistic_model = sklearn.linear_model.LogisticRegression(penalty='none', fit_intercept=False);
logistic_model.fit(X, y);
```

Check your answer by running the code cell below.

In [335…

```
assert 'logistic_model' in globals(), "You didn't create a variable named 'logistic_model'!"
assert isinstance(logistic_model, sklearn.linear_model.LogisticRegression), "Expected a LogisticRegression inst
assert hasattr(logistic_model, 'coef_'), "No model coefficients yet! You didn't fit the model to any data!"
assert logistic_model.intercept_ == 0.0, "You forgot to disable fitting of the intercept!"
assert np.allclose(logistic_model.coef_, [[18.5251137, 10.49283446]]), "The parameters seem incorrect! Not L-BF
print("Correct!")
```

```
Correct!
```

Notice that the model parameters (coefficients) found by the *LogisticRegression* are much larger than those found by your gradient descent solver. That is only because scikit-learn uses a more powerful optimization algorithm and can learn very sharp decision boundaries in fewer steps than mere gradient descent can. If you increase your *num_steps* argument your solver will find similarly large coefficients.

Plot several LogisticRegression predictions at once by running the code cell below.

In [336…

```
x0 = np.ones(50)                                 # A column of 1s so that the bias term w[0] gets added
x1 = np.linspace(-5, 5, 50)                      # A column of x values ranging from [-5, 5]
X_test = np.column_stack([x0, x1])               # A 20x2 matrix where X[i,:] is the ith x vector
y_test = logistic_model.predict_proba(X_test)    # Evaluate all x values and get two probabilities back (class 0,
plt.scatter(x1, y_test[:,1], 10, 'r')            # Plot probability of class 1 only
plt.scatter(X[:,1], y, edgecolor='b', facecolor='none')
plt.xlabel("$x_1$")
plt.ylabel("$y$")
plt.title("Sample predictions for LogisticRegression model");
```


In [ ]: