Lab 2 Exercises for COMP 6321 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 [372]:

```
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 [373]:

```
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 [374]:

```
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 [375]:

```
def eval_on_grid_vectorized(func, extent, numsteps):
    # Your code here. Aim for 4-6 lines.
    x1min, x1max, x2min, x2max = extent
    x = np.linspace(x1min, x1max, numsteps)
    y = np.linspace(x2min, x2max, numsteps)
    xv, yv = np.meshgrid(x, y)
    z = func(xv, yv)
    return xv, yv , z
```

Check your answer by running the code cell below.

In [376]:

```
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__ impor
t eval_on_grid_unvectorized, args", number=10)
vec_time   = timeit.timeit('eval_on_grid_vectorized(*args)',   setup="from __main__ impo
rt eval_on_grid_vectorized, args", number=10)
print("Your vectorized code ran %.1fx faster than the original code on a 200x200 grid" %
(unvec_time/vec_time))
```

```
Correct!
Your vectorized code ran 138.3x faster than the original code on a 200x200 grid
```

Exercise 1.2 — Plot a function as a heatmap

Consider the function

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

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 [377]:

```
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 [378]:

```
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!
```

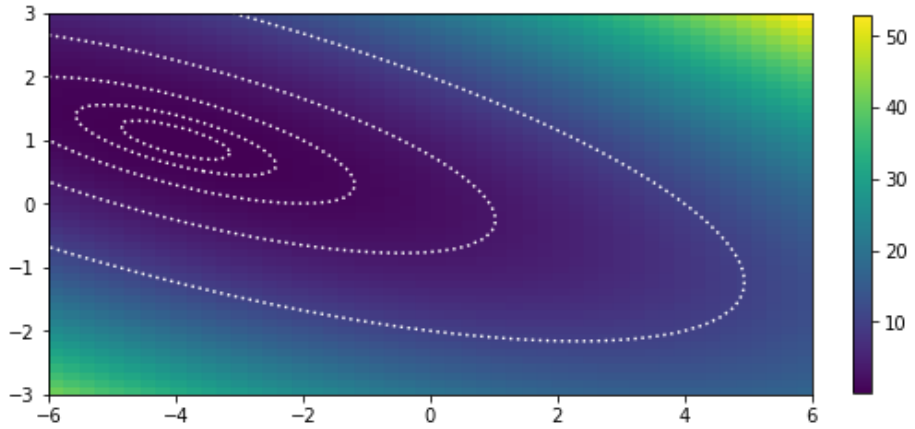
Write plotting code to visualize your $f(x_1, x_2)$ function over the interval $x_1 \in [-6, 6]$ and $x_2 \in [-3, 3]$. Your plot should look like this:

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 [ ]:

```
def plot_exercise12():
    # Your code here. Aim for 9-12 lines.
  x1, x2, y = eval_on_grid_vectorized(f, [-6 , 6,-3, 3], 50)
  plt.figure (num = None, figsize= (8,4))
  plt.imshow(y, origin='lower', extent=(x1.min(), x1.max(), x2.min(), x2.max()))
  plt.colorbar(fraction=0.046/2)
  plt.contour(x1, x2, y, np.logspace(-1 , 1, 5), colors="white", linestyles=":")


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 figure out the correct formulas to implement by yourself. Consider using *np.stack* to form the final array of gradients.

In [ ]:

```
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.
    a = (x1 + 2 * x2 + 2 )/2
    b = (4 * x2 + x1 )
    return np.stack([a,b])
```

Check your answer by running the code cell below.

In [ ]:

```
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!
```

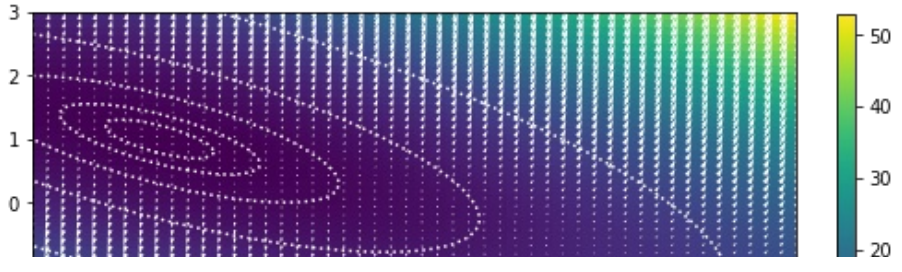
Write plotting code to overlay the gradient $\nabla f(x_1, x_2)$ over your figure from Exercise 1.2. Your plot should look like this:

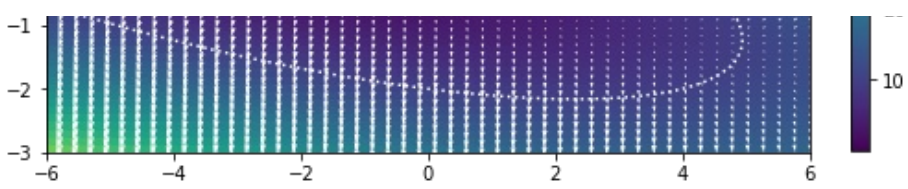
Specifically:

- **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 [263]:

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

    # Your code here. Aim for 2-4 lines.
    x1, x2, grad = eval_on_grid_vectorized(f_grad, [-6 , 6,-3, 3], 50)
    u, v = f_grad(x1,x2)
    plt.quiver(x1, x2, u,v, color='white')


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 [370]:

```
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.

    x_old = x_init
    for i in range(num_steps):
        x_old = x_old - learn_rate * f_grad(*x_old)
    return x_old
```

Check your answer by running the code cell below

In [371]:

```
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 val
ue!"
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 fe
w steps!"
print("Correct!")
```

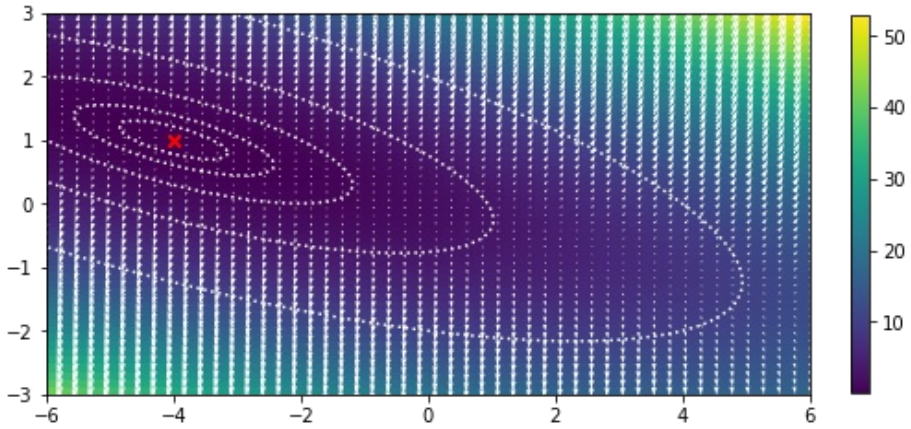
```
Correct!
```

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 [379]:

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

# Run gradient descent in chunks of 5 steps at a time, plotting the resulting 'x' after e
ach chunk
learn_rate = 0.05
x_init = np.array([-4, 1])
for num_steps in range(0, 250, 5):                              # Repeatedly run gradient
descent from the initial point,
```

```
    x = gradient_descent_on_f(x_init, learn_rate, num_steps)  # eventually running it fo
r 100 steps.
    plt.plot(*x, 'xr');                                       # Add a little 'x' to the plo
t to show how far it got.
```



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

$$\mathbf{x} = \begin{bmatrix} 1 & x_1 & \dots & x_D \end{bmatrix}^T$$
$$\mathbf{w} = \begin{bmatrix} w_0 & w_1 & \dots & w_D \end{bmatrix}^T$$

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:

```
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 $X^T \in \mathrm{R}^{(D+1)\times N}$ 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 $X \in \mathrm{R}^{N\times(D+1)}$ as an argument, you should figure out what mathematical expression would result in the $\hat{y} \in \mathrm{R}^N$ vector shown above. Hint: the solution is only a small change from `X.T @ w`.

In [380]:

```
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 [381]:

```
w = np.array([2, 0.5])                                  # Parameters corresponding to the 1D l
ine 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 again.")
w = np.array([1, 0.5, 0.25])                            # Parameters corresponding to the 2D p
lane y = 1 + 0.5*x1 + 0.25*x2
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!")
```

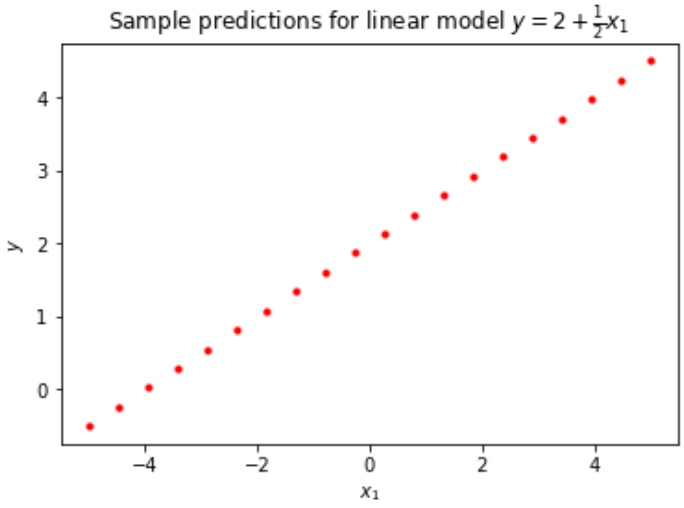
```
Correct!
```

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

In [ ]:

```
w = np.array([2, 0.5])              # Parameters corresponding to the 1D line y = 2 + 0.5*x
1
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 [285]:

```
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.
    w = w_init
    for i in range(num_steps):
        grad = X.T @ X @ w - X.T @ y
        w -= learn_rate * grad
    return w
```

Check your answer by running the code cell below.

In [286]:

```
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 [ ]:

```
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 @ X) @ X.T @ y
```

In [ ]:

```
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:

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

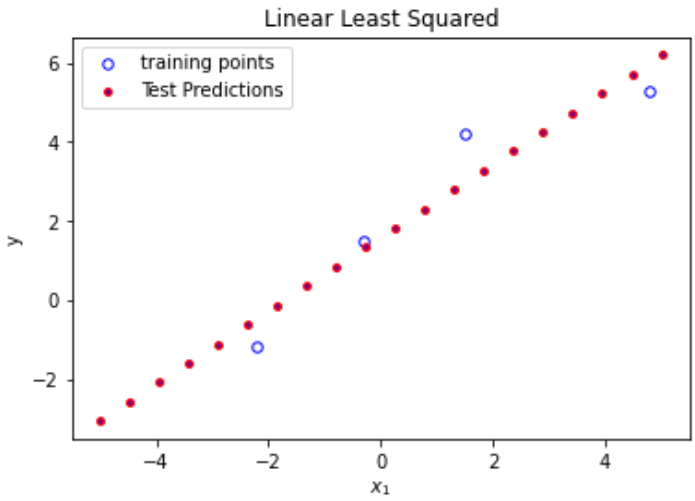
Write code to create the following plot:

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 [ ]:

```
# 1. Define the training set. Aim for 2 lines.
X = np.column_stack([np.ones((4, 1)), np.array([[-2.2], [-0.3], [1.5], [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[:, 1], y, s=30, facecolors='white', edgecolors='blue', marker='o', label='
training points')

# 3. Run linear least squares regression on the training set to compute 'w'. Aim for 1 li
ne.
w = linear_regression_by_direct_solve(X, y)

# 4. Define the test set matrix of shape (20,2). Aim for 1-3 lines.
x0 = np.ones((20, 1))
x1 = np.linspace(-5, 5, 20)
X_test = np.column_stack([x0, x1])

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

# 6. Plot the test predictions. Aim for 1 line, plus a few lines to configure the plot (a
xis labels etc).

plt.scatter(x1, y_test_predict, s=15, facecolors='purple', edgecolors='red', marker='o',
label='Test Predictions')
plt.xlabel("$x_1$")
plt.ylabel("y")
plt.title("Linear Least Squared")
plt.legend()
plt.show()
```



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 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 [ ]:

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

Out[ ]:

```
LinearRegression(copy_X=True, fit_intercept=False, n_jobs=None, normalize=False)
```

Check your answer by running the code cell below.

In [ ]:

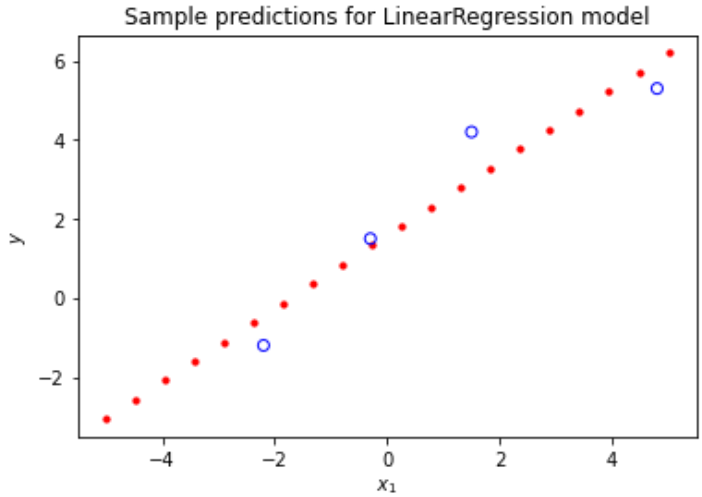
```
assert 'linear_model' in globals(), "You didn't create a variable named 'linear_model'!"
assert isinstance(linear_model, sklearn.linear_model.LinearRegression), "Expected a Line
arRegression instance!"
assert hasattr(linear_model, 'coef_'), "No model coefficients yet! You didn't fit the mod
el to 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 parameter
s you learned seem incorrect!"
print("Correct!")
```

```
Correct!
```

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

In [ ]:

```
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='blue', 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 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 [ ]:

```
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 [ ]:

```
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 + 1.5*x1)
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 again.")
w = np.array([1, 0.5, 0.25])                        # Parameters corresponding to the 2D plane y = 1 + 0.5*x1 + 0.25*x2
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!\n%s" % y
print("Correct!")
```

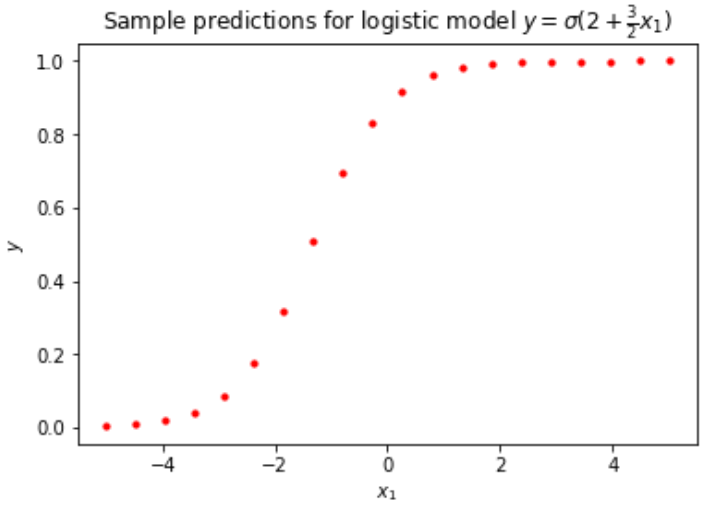
```
Correct!
```

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

In [ ]:

```
w = np.array([2, 1.5])                              # Parameters corresponding to logistic mode
```

```
l y = sigmoid(2 + 1.5*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_test = np.column_stack([x0, x1])              # A 20x2 matrix where X[i,:] is the ith x v
ector
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:

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

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

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

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 $i = 1, \ldots, N$).

In [ ]:

```
def logistic_regression_grad(X, y, w):
    """Returns the gradient for basic logistic regression."""
    # Your code here. Aim for 1-3 lines.
    sum = np.sum(X * (sigmoid(X @ w) - y).reshape(y.size, 1), axis=0)
    return sum

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 ta
rgets.
    """
    # Your code here. Aim for 4-5 lines.
    w = w_init
    for i in range(num_steps):
        grad = logistic_regression_grad(X, y.reshape(y.size, 1), w.reshape(w.size, 1))
        w = w - learn_rate * grad
    return w
```

Check your answer by running the code cell below.

In [ ]:

```
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.shap
e,)
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 s
eem 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:

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

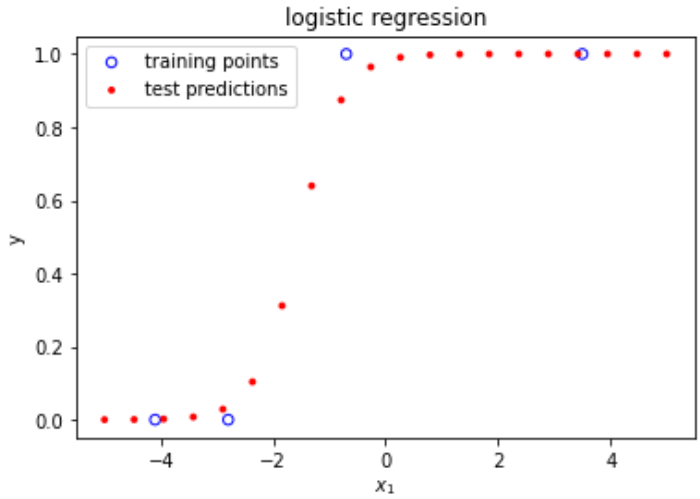
1. **Make ndarrays X and $\mathbf{y}$ that contain the above training set.**
2. **Plot the training set in blue. Use the x coordinates from the second column of X, ignoring the first column.**
3. **Run logistic regression on $(X, \mathbf{y})$ to get fitted parameters $\mathbf{w}$; use your *logistic_regression* 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 [ ]:

```
# 1. Define the training set. Aim for 2 lines.
X = np.column_stack([np.ones((4, 1)), np.array([[-4.1], [-2.8], [-0.7], [3.5]])])
y = np.array([[0], [0], [1], [1]])

# 2. Plot the training set. Aim for 1 line.
plt.scatter(X[:, 1], y, s=30, facecolors='none', edgecolors='blue', label='training poin
ts')

# 3. Run logistic regression on the training set to get 'w'. Aim for 1-2 lines.
w_init = np.array([0.0, 1.0])
w = logistic_regression(X, y, w_init)
# 4. Define the test set matrix of shape (20,2). Aim for 1-3 lines.

x0 = np.ones((20, 1))
x1 = np.linspace(-5, 5, 20).reshape(x1.size, 1)
X_test = np.column_stack([x0, x1])
# 5. Use the linear model to make predictions on the test set. Aim for 1 line.
y_test_predict = logistic_model_predict(X_test, w)
# 6. Plot the test predictions. Aim for 1 line, plus a few lines to configure the plot (a
xis labels etc).
plt.scatter(x1, y_test_predict, s=15, facecolors='red', edgecolors='none', label='test p
redictions')
plt.xlabel("$x_1$")
plt.ylabel("y")
plt.title("logistic regression")
plt.legend()
plt.show()
```



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 `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":

In [ ]:

```
# Your code here. Aim for 2 lines.
logistic_model = sklearn.linear_model.LogisticRegression(fit_intercept=False, penalty='no
ne')
logistic_model.fit(X, y)
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/utils/validation.py:760: DataConversionWar
ning: A column-vector y was passed when a 1d array was expected. Please change the shape
of y to (n_samples, ), for example using ravel().
  y = column_or_1d(y, warn=True)
```

Out[ ]:

```
LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=False,
                   intercept_scaling=1, l1_ratio=None, max_iter=100,
                   multi_class='auto', n_jobs=None, penalty='none',
                   random_state=None, solver='lbfgs', tol=0.0001, verbose=0,
                   warm_start=False)
```

Check your answer by running the code cell below.

In [ ]:

```
assert 'logistic_model' in globals(), "You didn't create a variable named 'logistic_mode
l'!"
assert isinstance(logistic_model, sklearn.linear_model.LogisticRegression), "Expected a
LogisticRegression instance!"
assert hasattr(logistic_model, 'coef_'), "No model coefficients yet! You didn't fit the m
odel 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 se
em incorrect! Not L-BFGS? Used penalty?"
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 [ ]:

```
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 probab
ilities back (class 0, class 1)
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");
```