# 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 [25]:
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 [26]:
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 [27]:
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 [28]:
def eval_on_grid_vectorized(func, extent, numsteps):
    x1min, x1max, x2min, x2max = extent
    x1, x2 = np.meshgrid(np.linspace(x1min, x1max, numsteps), np.linspace(x2min, x2ma
    y = func(x1, x2)
    return x1, x2, y
```

**Check your answer** by running the code cell below.

```
In [29]:
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__ i
vec_time   = timeit.timeit('eval_on_grid_vectorized(*args)',   setup="from __main__ i
print("Your vectorized code ran %.1fx faster than the original code on a 200x200 grid"

Correct!
Your vectorized code ran 299.1x 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 [30]:
def f(x1, x2):
    return (((1 / 2) * x1 + x2 + 1) ** 2) + ((x2 - 1) ** 2)
```

**Check your answer** by running the code cell below.

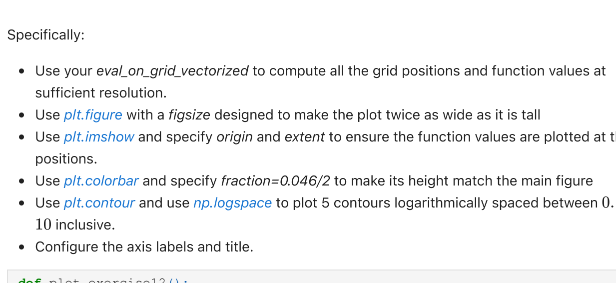
```
In [31]:
v = f(2.5, -4.0)
assert isinstance(v, float), "Expected float args to give float result"
assert v == 28.0625, "Wrong return value for float"
v = f(np.eye(3, 4), np.arange(12).reshape(3, 4))
assert isinstance(v, np.ndarray), "Expected ndarray args to give ndarray result"
np.testing.assert_equal(v, [[3.25, 4., 10., 20.], [34., 58.25, 74., 100.], [130., 164
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 [32]:
def plot_exercise12():
    extent = (-6, 6, -3, 3)
    x1, x2, y = eval_on_grid_vectorized(f, extent, 100)

    plt.figure(figsize=(10, 5))
    plt.imshow(y, extent=extent, origin="lower")

    plt.colorbar(fraction=0.046/2)
    plt.contour(x1, x2, y, levels=np.logspace(-1, 1, 5), colors="white", linestyles="

    plt.xlabel("$x_1$")
    plt.ylabel("$x_2$")
    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 [33]:
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,...).
    """
    x1, x2 = x1/2 + x2 + 1, x1 + 4 * x2
    return np.stack((x1, x2))
```

**Check your answer** by running the code cell below.

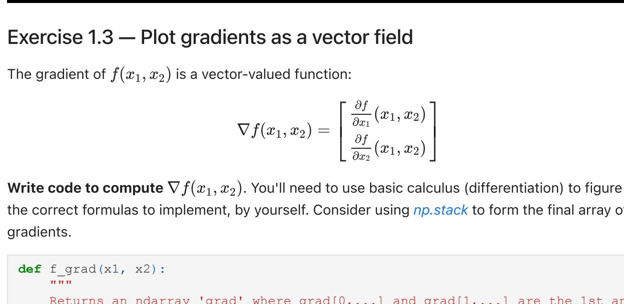
```
In [34]:
v = f_grad(3.5, -15.0)
assert isinstance(v, np.ndarray), "Expected float args to give ndarray result"
np.testing.assert_equal(v, [-12.25, -56.5])
v = f_grad(np.eye(3, 4), np.arange(12).reshape(3, 4))
assert isinstance(v, np.ndarray), "Expected array args to give ndarray result"
assert v.shape == (2, 3, 4), "Result was wrong shape"
np.testing.assert_equal(v, [[[ 1.5,  2. ,  3. ,  4. ], [ 5. ,  6.5,  7. ,  8. ], [ 9.
                           [[ 1. ,  4. ,  8. , 12. ], [16. , 21. , 24. , 28. ], [32.
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 [35]:
def plot_exercise13():
    plot_exercise12()  # Start with your previous plot

    x1, x2, y = eval_on_grid_vectorized(f_grad, (-6, 6, -3, 3), 25)
    plt.quiver(x1, x2, y[0], y[1], 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.

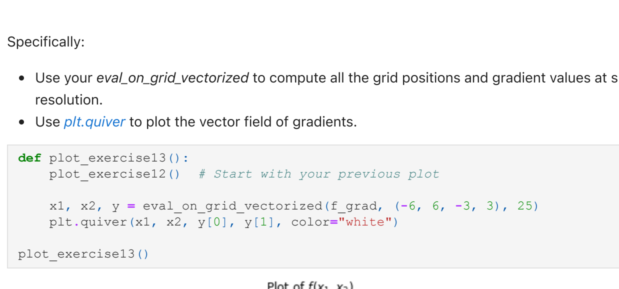
```
In [36]:
def gradient_descent_on_f(x_init, learn_rate, num_steps):
    """
    Runs num_steps of gradient descent from point x_init using
    the given learning rate, and returns the new x coordinate.
    Here x_init is an ndarray with shape (2,).
    """
    for _ in range(num_steps):
        x_init = 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 [37]:
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
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
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 [38]:
plot_exercise13()  # Plot the vector field first

# Run gradient descent in chunks of 5 steps at a time, plotting the resulting 'x' aft
learn_rate = 0.05
x_init = np.array([2.0, 1.0])                       # Start from initial poin
for num_steps in range(0, 250, 5):                  # Repeatedly run gradien
    x = gradient_descent_on_f(x_init, learn_rate, num_steps)  # eventually running it
    plt.plot(*x, 'xr');                             # Add a little 'x' to the p
```



*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

$$\mathbf{x} = [1 \quad x_1 \quad \ldots \quad x_D]^T \tag{1}$$
$$\mathbf{w} = [w_0 \quad w_1 \quad \ldots \quad w_D]^T \tag{2}$$

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:

```
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`.

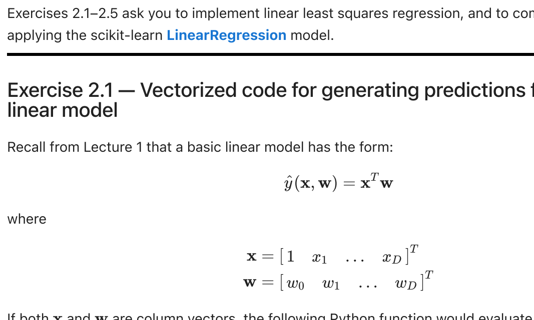
```
In [39]:
def linear_model_predict(X, w):
    """
    Returns predictions from linear model y(x, w) at each point X[i,:] using parame
    Given X with shape (N,D+1), w must have shape (D+1,) and the result will have sha
    """
    return X @ w
```

**Check your answer** by running the code cell below.

```
In [40]:
w = np.array([2, 0.5])                          # Parameters corresponding to the 1
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 i
w = np.array([1, 0.5, 0.25])                    # Parameters corresponding to the 2
X = np.array([[1., -3., 1.], [1., 3., 0.], [1., 5., -2.]])  # Evaluate at differen
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 fea
print("Correct!")

Correct!
```

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

```
In [41]:
w = np.array([2, 0.5])          # Parameters corresponding to the 1D line y = 2 + 0.
x0 = np.ones(20)                # A column of 1s so that the bias term w[0] gets add
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("$y$")
[illegible]
```



[illegible]

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 [42]:
def linear_regression_by_gradient_descent(X, y, w_init, learn_rate=0.05, num_steps=50
    """
    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.
    """
    for _ in range(num_steps):
        loss = ((X.T @ X) @ w_init) - (X.T @ y)
        w_init -= learn_rate * loss
    return w_init
```

**Check your answer** by running the code cell below.

```
In [43]:
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 [44]:
def linear_regression_by_direct_solve(X, y):
    """Fits a linear model by directly solving for the optimal parameter vector w."""
    return np.linalg.inv(X.T @ X) @ X.T @ y
```

```
In [45]:
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:

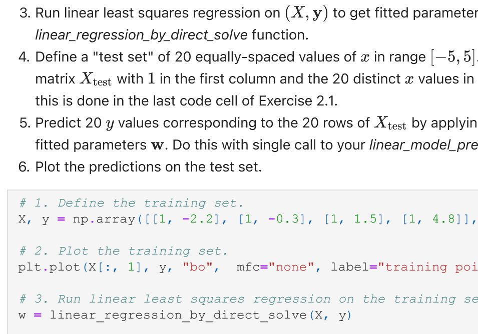
$$X = \begin{bmatrix} 1 & -2.2 \\ 1 & -0.3 \\ 1 & 1.5 \\ 1 & 4.8 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} -1.2 \\ 1.5 \\ 4.2 \\ 5.3 \end{bmatrix}$$

**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 $X_{\text{test}}$ 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 $X_{\text{test}}$ 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 [46]:
# 1. Define the training set.
X, y = np.array([[1, -2.2], [1, -0.3], [1, 1.5], [1, 4.8]], dtype="float64"), np.array

# 2. Plot the training set.
plt.plot(X[:, 1], y, "bo",  mfc="none", label="training points")

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

# 4. Define the test set matrix of shape (20,2).
x0, x1 = np.ones(20), np.linspace(-5, 5, 20)
test_set = np.vstack((x0, x1)).T

# 5. Use the linear model to make predictions on the test set.
prediction = linear_model_predict(test_set, w)

# 6. Plot the test predictions.
plt.plot(x1, prediction, "r.", label="prediction")
plt.legend()
plt.xlabel("$x_1$")
plt.ylabel("$y$")
plt.title("linear least squares regression")

Out[46]: Text(0.5, 1.0, 'linear least squares 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.

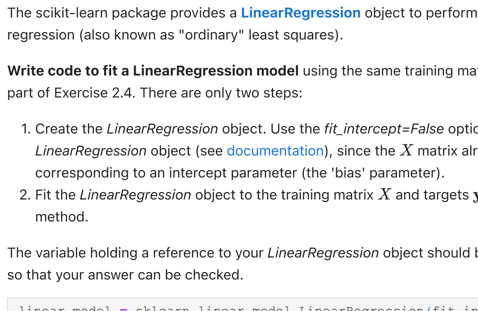
```
In [47]:
linear_model = sklearn.linear_model.LinearRegression(fit_intercept=False)
linear_model.fit(X, y)

Out[47]: LinearRegression(fit_intercept=False)
```

**Check your answer** by running the code cell below.

```
In [48]:
assert 'linear_model' in globals(), "You didn't create a variable named 'linear_model
assert isinstance(linear_model, sklearn.linear_model.LinearRegression), "Expected a L
assert hasattr(linear_model, 'coef_'), "No model coefficients yet! You didn't fit the
assert linear_model.intercept_ == 0.0, "You forgot to disable fitting of the intercep
assert np.allclose(linear_model.coef_, [[1.57104472, 0.92521608]]), "The model paramet
print("Correct!")

Correct!
```

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

```
In [49]:
x0 = np.ones(20)                        # A column of 1s so that the bias term w[0] ge
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 vec
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.

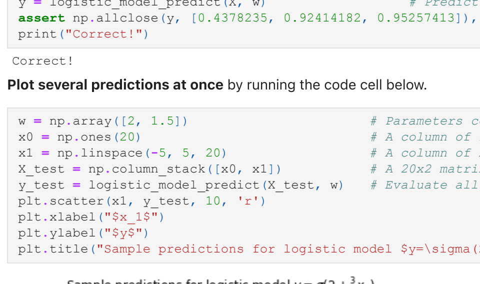
```
In [50]:
def sigmoid(z):
    """Returns the element-wise logistic sigmoid of z."""
    return 1 / (1 + np.exp(-z))

def logistic_model_predict(X, w):
    """
    Returns predictions from logistic model y(x, w) at each point X[i,:] using paramet
    Given X with shape (N,D+1), w must have shape (D+1,) and the result will have shap
    """
    return 1 / (1 + np.exp(-(X @ w)))
```

**Check your answer** by running the code cell below.

```
In [51]:
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
w = np.array([2, 1.5])                          # Parameters corresponding to logisti
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
w = np.array([1, 0.5, 0.25])                    # Parameters corresponding to the 2D
X = np.array([[1., -3., 1.], [1., 3., 0.], [1., 5., -2.]])  # Evaluate at differen
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-
print("Correct!")

Correct!
```

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

```
In [52]:
w = np.array([2, 1.5])                          # Parameters corresponding to logistic m
x0 = np.ones(20)                                # A column of 1s so that the bias term w
x1 = np.linspace(-5, 5, 20)                     # A column of x values ranging from [-5,
X_test = np.column_stack([x0, x1])              # A 20x2 matrix where X[i,:] is the ith
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 $i = 1, \ldots, N$).

```
In [53]:
def logistic_regression_grad(X, y, w):
    """Returns the gradient for basic logistic regression."""
    return (sigmoid(X @ w) - y) @ X

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
    """
    for _ in range(num_steps):
        w_init -= learn_rate * logistic_regression_grad(X, y, w_init)
    return w_init
```

**Check your answer** by running the code cell below.

```
In [54]:
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.
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" %
assert np.allclose(w, [-4.14100532, 2.95489589]), "Parameters found by gradient descen
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:

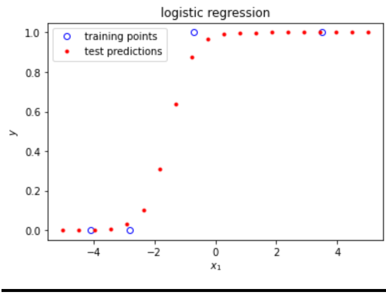
$$X = \begin{bmatrix} 1 & -4.1 \\ 1 & -2.8 \\ 1 & -0.7 \\ 1 & 3.5 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

**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 $X_{\text{test}}$ 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 $X_{\text{test}}$ 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 [55]:
# 1. Define the training set.
X, y = np.array([[1, -4.1], [1, -2.8], [1, -0.7], [1, 3.5]], dtype="float64"), np.arra

# 2. Plot the training set.
plt.plot(X[:, 1], y, "bo",  mfc="none", label="training points")

# 3. Run logistic regression on the training set to get 'w'.
w = logistic_regression(X, y, w_init=np.array([0.0, 1.0], dtype="float64"))

# 4. Define the test set matrix of shape (20,2).
x0, x1 = np.ones(20), np.linspace(-5, 5, 20)
test_set = np.vstack((x0, x1)).T

# 5. Use the linear model to make predictions on the test set.
predictions = logistic_model_predict(test_set, w)

# 6. Plot the test predictions.
plt.plot(x1, predictions, "r.", label="test predictions")
plt.legend()
plt.xlabel("$x_1$")
plt.ylabel("$y$")
plt.title("logistic regression")

Out[55]: Text(0.5, 1.0, 'logistic regression')
```




---

## 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 [56]:
```
logistic_model = sklearn.linear_model.LogisticRegression(fit_intercept=False, penalty=
logistic_model.fit(X, y)
```

Out[56]:
```
LogisticRegression(fit_intercept=False, penalty='none')
```

**Check your answer** by running the code cell below.

In [57]:
```
assert 'logistic_model' in globals(), "You didn't create a variable named 'logistic_mo
assert isinstance(logistic_model, sklearn.linear_model.LogisticRegression), "Expected
assert hasattr(logistic_model, 'coef_'), "No model coefficients yet! You didn't fit th
assert logistic_model.intercept_ == 0.0, "You forgot to disable fitting of the interce
assert np.allclose(logistic_model.coef_, [[18.5251137, 10.49283446]]), "The parameters
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 [58]:
```
x0 = np.ones(50)                                   # A column of 1s so that the bias term
x1 = np.linspace(-5, 5, 50)                        # A column of x values ranging from [-
X_test = np.column_stack([x0, x1])                 # A 20x2 matrix where X[i,:] is the ith
y_test = logistic_model.predict_proba(X_test)      # Evaluate all x values and get two pro
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");
```