Worksheet 21

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Topics

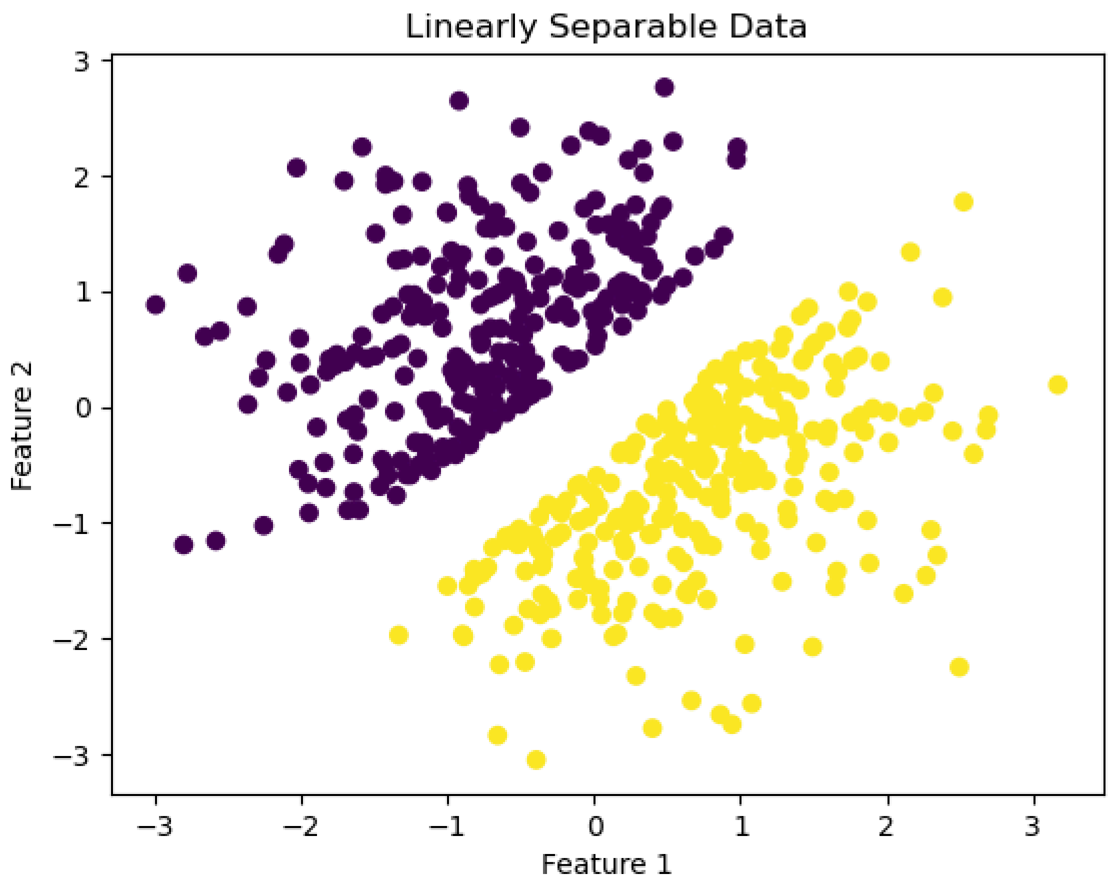
- Logistic Regression
- Gradient Descent

Logistic Regression

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import sklearn.datasets as datasets
from sklearn.pipeline import make_pipeline
from sklearn.linear_model import LogisticRegression
from sklearn.preprocessing import PolynomialFeatures

centers = [[0, 0]]
t, _ = datasets.make_blobs(n_samples=750, centers=centers, cluster_std=1

# LINE
def generate_line_data():
    # create some space between the classes
    X = np.array(list(filter(lambda x : x[0] - x[1] < -.5 or x[0] - x[1]
    Y = np.array([1 if x[0] - x[1] >= 0 else 0 for x in X])
    return X, Y

# CIRCLE
def generate_circle_data(t):
    # create some space between the classes
    X = np.array(list(filter(lambda x : (x[0] - centers[0][0])**2 + (x[1
    Y = np.array([1 if (x[0] - centers[0][0])**2 + (x[1] - centers[0][1]
    return X, Y

# XOR
def generate_xor_data():
    X = np.array([
        [0,0],
        [0,1],
        [1,0],
        [1,1]])
    Y = np.array([x[0]^x[1] for x in X])
    return X, Y
```

a) Using the above code, generate and plot data that is linearly separable.

In [2]:
```
X, Y = generate_line_data()

plt.scatter(X[:, 0], X[:, 1], c=Y)
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.title('Linearly Separable Data')
plt.show()
```



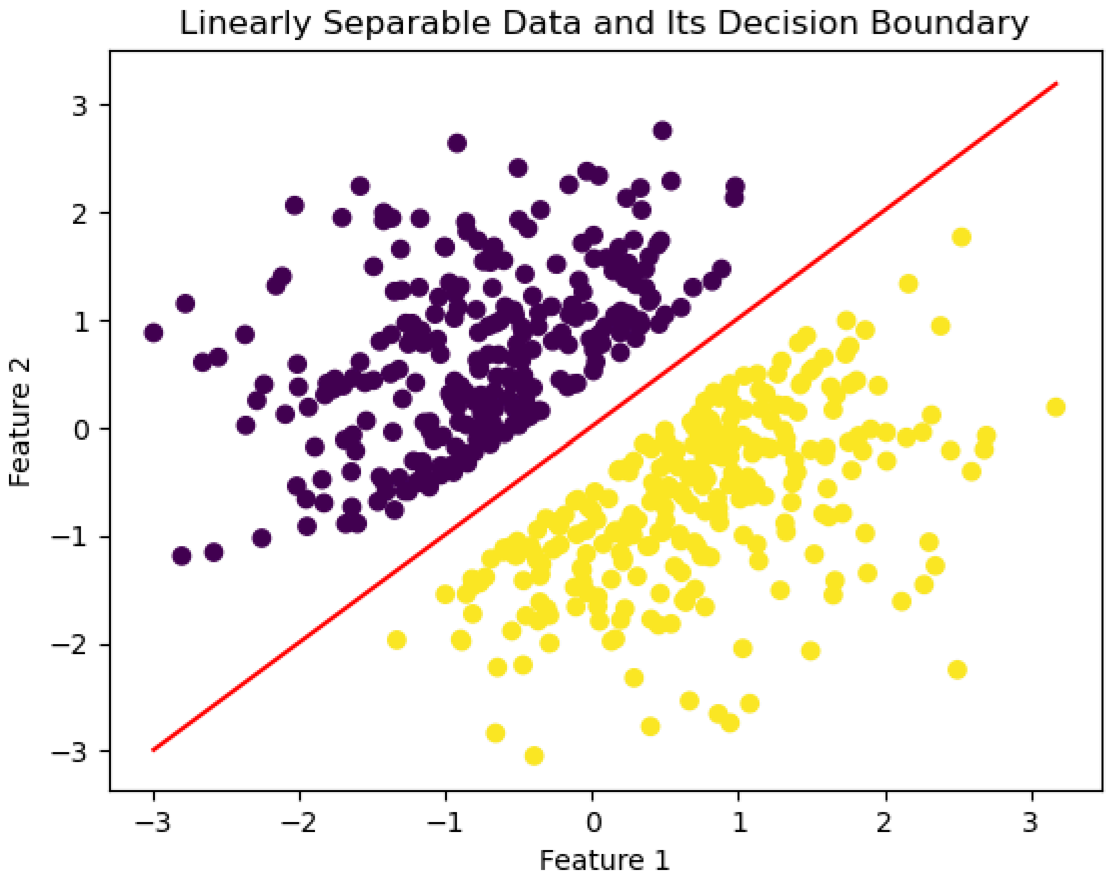
b) Fit a logistic regression model to the data a print out the coefficients.

In [3]:
```
model = LogisticRegression().fit(X, Y)
print(f"coefficients: {model.coef_[0]}")
print(f"intercept: {model.intercept_}")
```

```
coefficients: [ 4.11337993 -4.10105513]
intercept: [0.05839469]
```

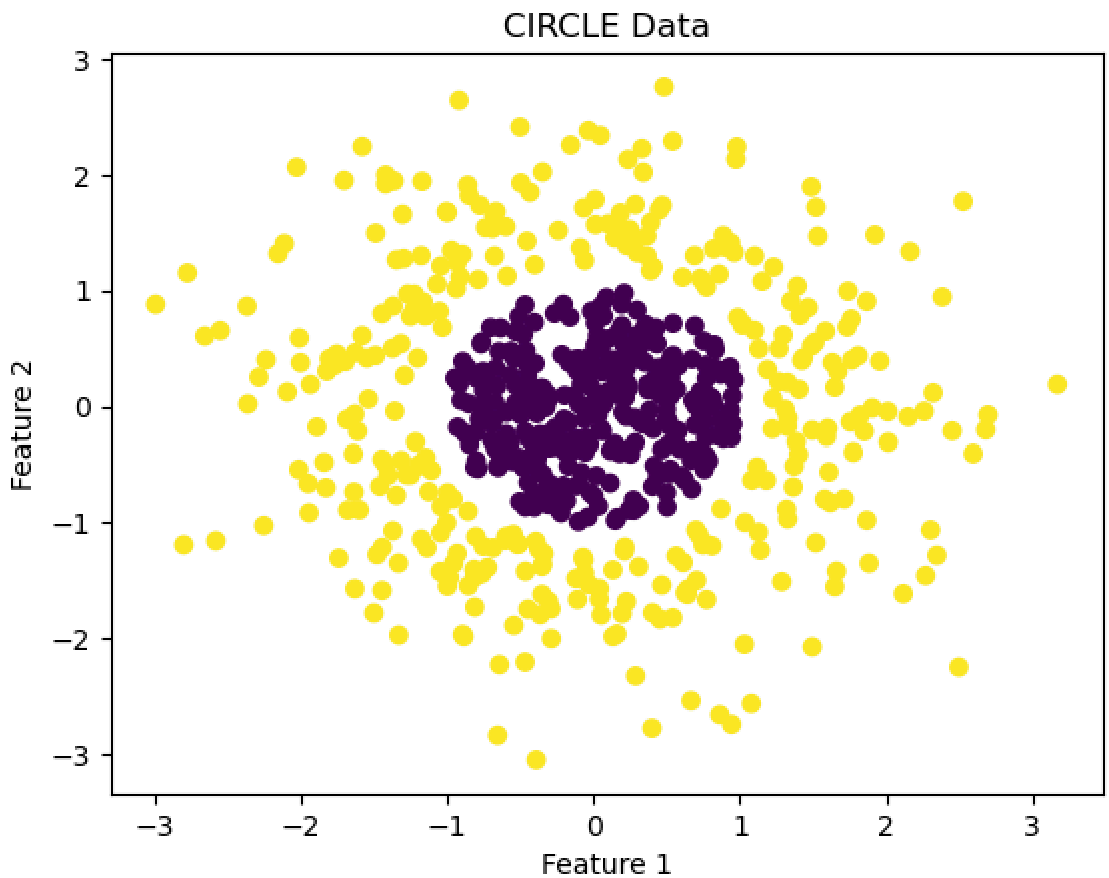
c) Using the coefficients, plot the line through the scatter plot you created in a). (Note: you need to do some math to get the line in the right form)

In [4]:
```
x_values = np.linspace(np.min(X[:, 0]), np.max(X[:, 0]), 10)
y_values = -(model.coef_[0][0]/model.coef_[0][1]) * x_values - model.int

plt.scatter(X[:, 0], X[:, 1], c=Y)
plt.plot(x_values, y_values, c='r')
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.title('Linearly Separable Data and Its Decision Boundary')
plt.show()
```



d) Using the above code, generate and plot the CIRCLE data.

In [5]:
```
X, Y = generate_circle_data(t)

plt.scatter(X[:, 0], X[:, 1], c=Y)
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.title('CIRCLE Data')
plt.show()
```



e) Notice that the equation of an ellipse is of the form $$ax^2 + by^2 = c$$

Fit a logistic regression model to an appropriate transformation of X.

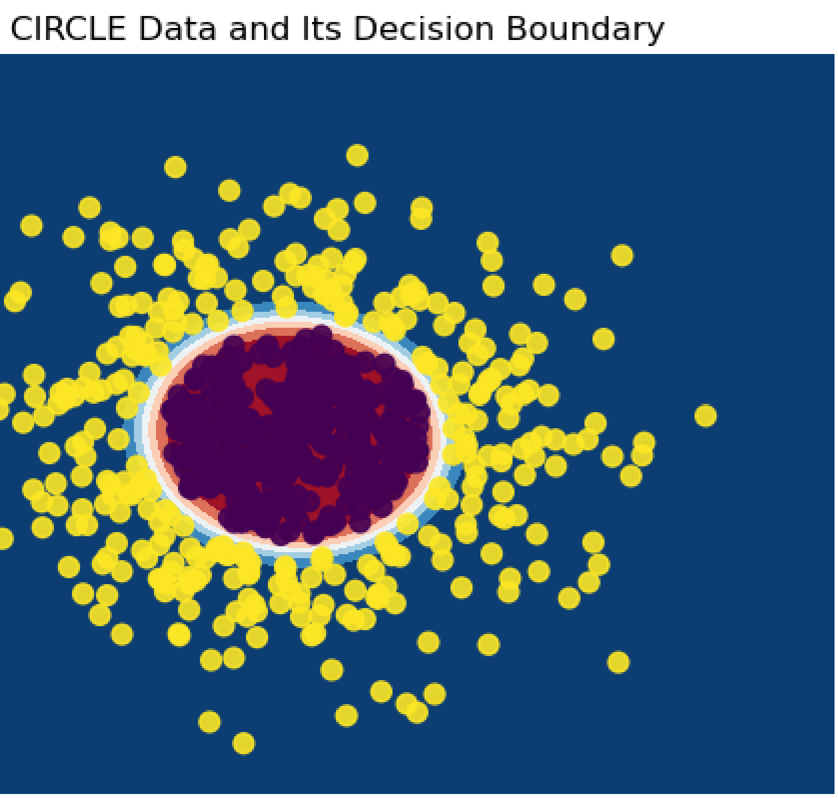
In [6]:
```
poly = PolynomialFeatures(degree=2, include_bias=False)
lr = LogisticRegression()
model = make_pipeline(poly, lr).fit(X, Y)
print(f"coefficients: {lr.coef_[0]}")   # x, y, x^2, xy, y^2
print(f"intercept: {lr.intercept_}")
```

```
coefficients: [ 0.02985162 -0.04753247  4.90954898  0.37928     4.95645
605]
intercept: [-6.47659385]
```

f) Plot the decision boundary using the code below.

In [7]:
```python
# create a mesh to plot in
h = .02  # step size in the mesh
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
meshData = np.c_[xx.ravel(), yy.ravel()]

fig, ax = plt.subplots()
A = model.predict_proba(meshData)[:, 1].reshape(xx.shape)
Z = model.predict(meshData).reshape(xx.shape)
ax.contourf(xx, yy, A, cmap="RdBu", vmin=0, vmax=1)
ax.axis('off')

# plot also the training points
ax.scatter(X[:, 0], X[:, 1], c=Y, s=50, alpha=0.9)
plt.title('CIRCLE Data and Its Decision Boundary')
```

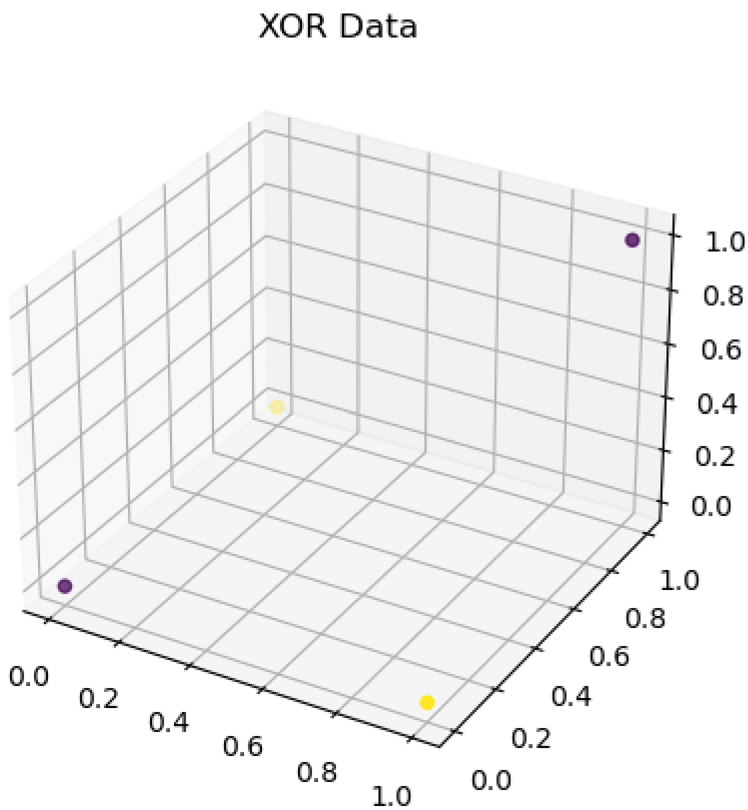
Out[7]:
```
Text(0.5, 1.0, 'CIRCLE Data and Its Decision Boundary')
```



g) Plot the XOR data. In this 2D space, the data is not linearly separable, but by introducing a new feature $$x_3 = x_1 * x_2$$

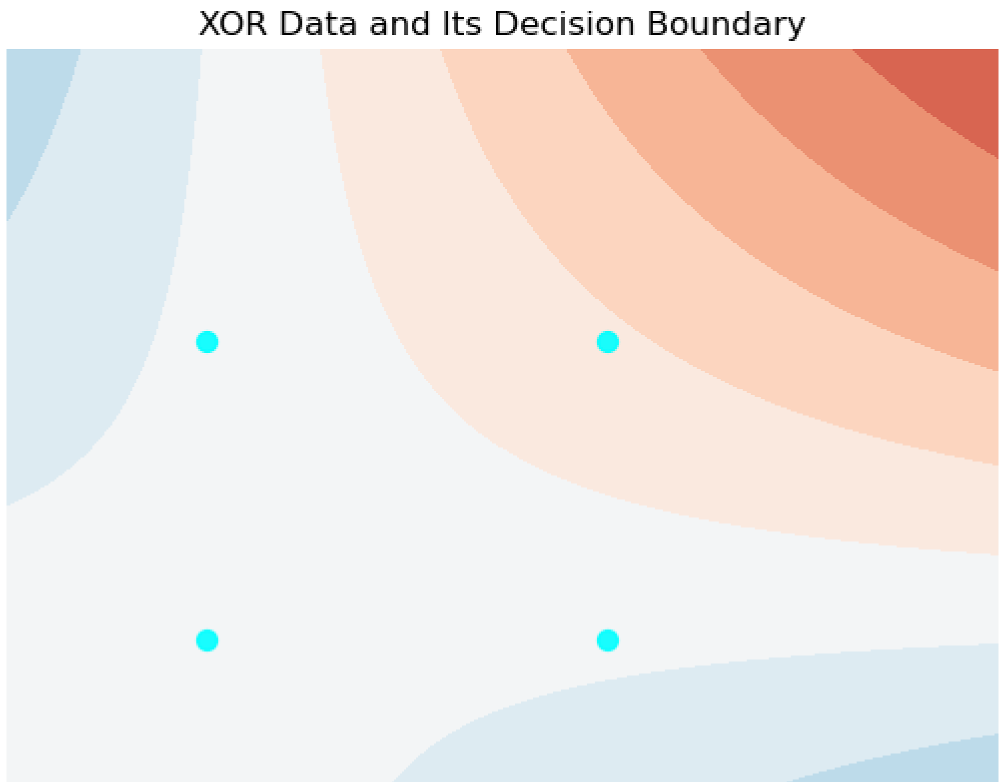
(called an interaction term) we should be able to find a hyperplane that separates the data in 3D. Plot this new dataset in 3D.

In [8]:
```
from mpl_toolkits.mplot3d import Axes3D

X, Y = generate_xor_data()
ax = plt.axes(projection='3d')
ax.scatter3D(X[:, 0], X[:, 1], X[:, 0]*X[:, 1], c=Y)
plt.title('XOR Data')
plt.show()
```



h) Apply a logistic regression model using the interaction term. Plot the decision boundary.

In [9]:
```
poly = PolynomialFeatures(interaction_only=True)
lr = LogisticRegression(verbose=0)
model = make_pipeline(poly, lr).fit(X, Y)

# create a mesh to plot in
h = .02  # step size in the mesh
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
meshData = np.c_[xx.ravel(), yy.ravel()]

fig, ax = plt.subplots()
A = model.predict_proba(meshData)[:, 1].reshape(xx.shape)
Z = model.predict(meshData).reshape(xx.shape)
ax.contourf(xx, yy, A, cmap="RdBu", vmin=0, vmax=1)
ax.axis('off')

# plot also the training points
ax.scatter(X[:, 0], X[:, 1], color=Y, s=50, alpha=0.9)
plt.title('XOR Data and Its Decision Boundary')
plt.show()
```



In [10]:

```
%matplotlib widget
for i in range(20000):
    for solver in ['lbfgs', 'liblinear', 'newton-cg', 'newton-cholesky',
        X_transform = PolynomialFeatures(interaction_only=True, include_
        model = LogisticRegression(verbose=0, solver=solver, random_stat
        model.fit(X_transform, Y)
        print(model.score(X_transform, Y))
        if model.score(X_transform, Y) > .75:
            print("random state = ", i)
            print("solver = ", solver)
            break

print(model.coef_)
print(model.intercept_)

xx, yy = np.meshgrid([x / 10 for x in range(-1, 11)], [x / 10 for x in ra
z = - model.intercept_ / model.coef_[0][2] - model.coef_[0][0] * xx / mo

ax = plt.axes(projection='3d')
ax.scatter3D(X[: , 0], X[: , 1], X[: , 0]* X[: , 1], c=Y)
ax.plot_surface(xx, yy, z, alpha=0.5)
plt.show()
```

```
0.75
0.75
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0.75
0.75
0.75
```

i) Using the code below that generates 3 concentric circles, fit a logisitc regression model to it and plot the decision boundary.

In [11]:
```
t, _ = datasets.make_blobs(n_samples=1500, centers=centers, cluster_std=
                                random_state=0)

# CIRCLES
def generate_circles_data(t):
    def label(x):
        if x[0]**2 + x[1]**2 >= 2 and x[0]**2 + x[1]**2 < 8:
            return 1
        if x[0]**2 + x[1]**2 >= 8:
            return 2
        return 0
    # create some space between the classes
    X = np.array(list(filter(lambda x : (x[0]**2 + x[1]**2 < 1.8 or x[0]
    Y = np.array([label(x) for x in X])
    return X, Y

X, Y = generate_circles_data(t)

poly = PolynomialFeatures(2)
lr = LogisticRegression(max_iter=500, verbose=2)
model = make_pipeline(poly, lr).fit(X, Y)

# create a mesh to plot in
h = .02
x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max,
meshData = np.c_[xx.ravel(), yy.ravel()]

Z = model.predict(meshData).reshape(xx.shape)

fig, ax = plt.subplots()
ax.contourf(xx, yy, Z, cmap='RdBu', vmin=0, vmax=1, alpha=0.5)
ax.axis('off')
# plot also the training points
scatter = ax.scatter(X[:, 0], X[:, 1], c=Y, s=20, alpha=0.9)
plt.title('Concentric Data and Its Decision Boundary')
plt.show()
```

```
[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent
workers.
 This problem is unconstrained.
[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:    0.0s remaining:
0.0s
[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:    0.0s finished
```

```
RUNNING THE L-BFGS-B CODE
```

Gradient Descent

Recall in Linear Regression we are trying to find the line $$y = X \beta$$ that minimizes the sum of square distances between the predicted `y` and the `y` we observed in our dataset:

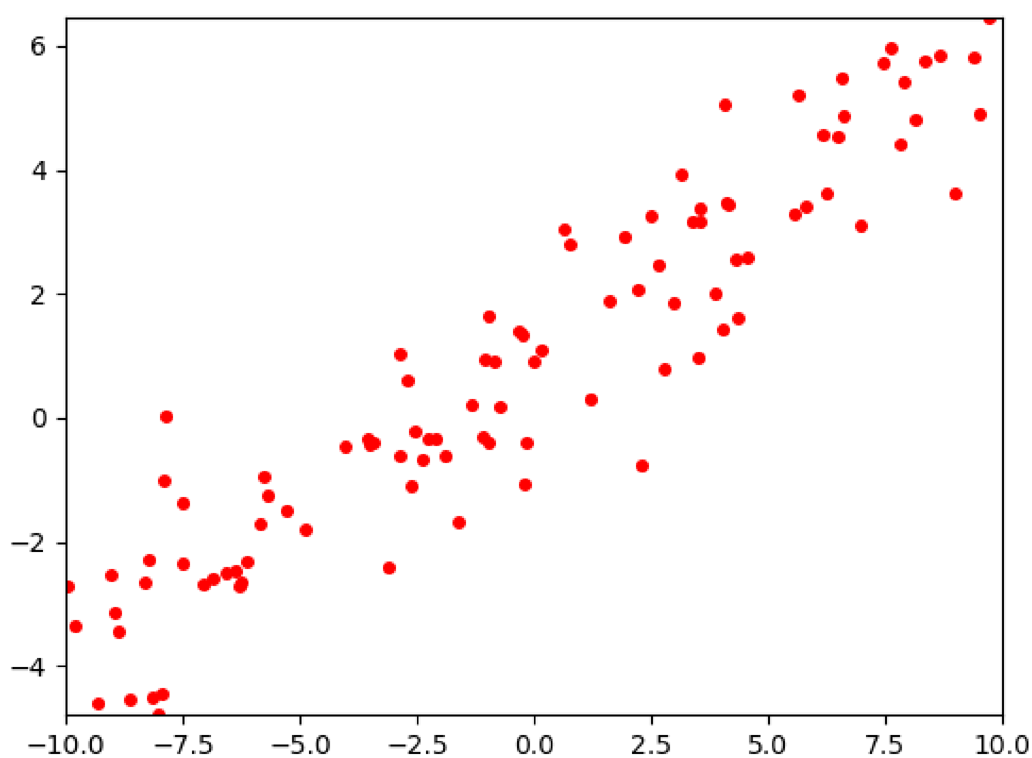
$$\mathcal{L}(\mathbf{\beta}) = \Vert \mathbf{y} - X\mathbf{\beta} \Vert^2$$

We were able to find a global minimum to this loss function but we will try to apply gradient descent to find that same solution.

a) Implement the `loss` function to complete the code and plot the loss as a function of beta.

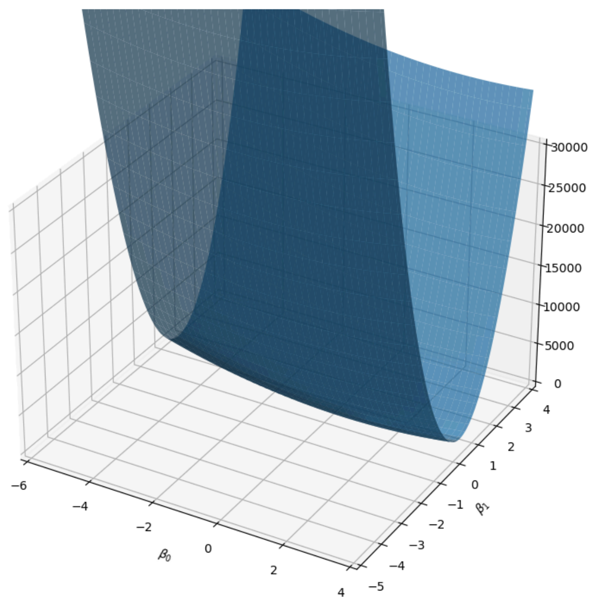
In [12]:
```
%matplotlib widget
from mpl_toolkits import mplot3d
import numpy as np
import matplotlib.pyplot as plt

beta = np.array([ 1 , .5 ])
xlin = -10.0 + 20.0 * np.random.random(100)
X = np.column_stack([np.ones((len(xlin), 1)), xlin])
y = beta[0]+(beta[1]*xlin)+np.random.randn(100)

fig, ax = plt.subplots()
ax.plot(xlin, y,'ro',markersize=4)
ax.set_xlim(-10, 10)
ax.set_ylim(min(y), max(y))
plt.show()
```

Figure



In [13]:
```
b0 = np.arange(-5, 4, 0.1)
b1 = np.arange(-5, 4, 0.1)
b0, b1 = np.meshgrid(b0, b1)

def loss(X, y, beta):
    return np.sum((y - X @ beta) ** 2)
def get_cost(B0, B1):
    res = []
    for b0, b1 in zip(B0, B1):
        line = []
        for i in range(len(b0)):
            beta = np.array([b0[i], b1[i]])
            line.append(loss(X, y, beta))
        res.append(line)
    return np.array(res)

cost = get_cost(b0, b1)

# Creating figure
fig = plt.figure(figsize =(14, 9))
ax = plt.axes(projection ='3d')
ax.set_xlim(-6, 4)
ax.set_xlabel(r'$\beta_0$')
ax.set_ylabel(r'$\beta_1$')
ax.set_ylim(-5, 4)
ax.set_zlim(0, 30000)

# Creating plot
ax.plot_surface(b0, b1, cost, alpha=.7)

# show plot
plt.show()
```

Figure



Since the loss is

$$\mathcal{L}(\mathbf{\beta}) = \Vert \mathbf{y} - X\mathbf{\beta} \Vert^2 = \beta^T X^T X \beta - 2\mathbf{\beta}^TX^T\mathbf{y} + \mathbf{y}^T\mathbf{y}$$

The gradient is

$$\nabla_\beta \mathcal{L}(\mathbf{\beta}) = 2X^T X \beta - 2X^T\mathbf{y}$$

b) Implement the gradient function below and complete the gradient descent algorithm

In [18]:
```
import numpy as np
from PIL import Image as im
import matplotlib.pyplot as plt

TEMPFILE = "temp.png"

def snap(betas, losses):
    # Creating figure
    fig = plt.figure(figsize=(14, 9))
    ax = plt.axes(projection='3d')
    ax.view_init(20, -20)
    ax.set_xlim(-5, 4)
    ax.set_xlabel(r'$\beta_0$')
    ax.set_ylabel(r'$\beta_1$')
    ax.set_ylim(-5, 4)
    ax.set_zlim(0, 30000)

    # Creating plot
    ax.plot_surface(b0, b1, cost, color='b', alpha=.7)
    ax.plot(np.array(betas)[:,0], np.array(betas)[:,1], losses, 'o-', c=
    fig.savefig(TEMPFILE)
    plt.close()
    return im.fromarray(np.asarray(im.open(TEMPFILE)))


def gradient(X, y, beta):
    return 2 * X.T @ X @ beta - 2 * X.T @ y


def gradient_descent(X, y, beta_hat, learning_rate, epochs, images):
    losses = [loss(X, y, beta_hat)]
    betas = [beta_hat]

    for _ in range(epochs):
        images.append(snap(betas, losses))
        beta_hat = beta_hat - learning_rate * gradient(X, y, beta_hat)

        losses.append(loss(X, y, beta_hat))
        betas.append(beta_hat)

    return np.array(betas), np.array(losses)


beta_start = np.array([-5, -2])
learning_rate = 0.0002  # try .0005
# learning_rate = 0.0005  # too large
images = []
betas, losses = gradient_descent(X, y, beta_start, learning_rate, 10, ima

images[0].save(
    'gd.gif',
    optimize=False,
    save_all=True,
    append_images=images[1:],
    loop=0,
    duration=500
```

```
)
```

c) Use the code above to create an animation of the linear model learned at every epoch.

In [20]:

```
def snap_model(beta):
    xplot = np.linspace(-10, 10, 50)
    yestplot = beta[0] + beta[1] * xplot
    fig, ax = plt.subplots()
    ax.plot(xplot, yestplot, 'b-', lw=2)
    ax.plot(xlin, y, 'ro', markersize=4)
    ax.set_xlim(-10, 10)
    ax.set_ylim(min(y), max(y))
    fig.savefig(TEMPFILE)
    plt.close()
    return im.fromarray(np.asarray(im.open(TEMPFILE)))


def gradient_descent(X, y, beta_hat, learning_rate, epochs, images):
    losses = [loss(X, y, beta_hat)]
    betas = [beta_hat]

    for _ in range(epochs):
        images.append(snap_model(beta_hat))
        beta_hat = beta_hat - learning_rate * gradient(X, y, beta_hat)

        losses.append(loss(X, y, beta_hat))
        betas.append(beta_hat)

    return np.array(betas), np.array(losses)


images = []
betas, losses = gradient_descent(X, y, beta_start, learning_rate, 100, i

images[0].save(
    'model.gif',
    optimize=False,
    save_all=True,
    append_images=images[1:],
    loop=0,
    duration=200
)
```

In logistic regression, the `loss` is the negative log-likelihood

$$ \mathcal{l}(\mathbf{\beta}) = - \frac{1}{N} \sum_{i=1}^{N} y_i \log(\sigma(x_i \beta)) + (1 - y_i)\log(1 - \sigma(x_i \beta))$$

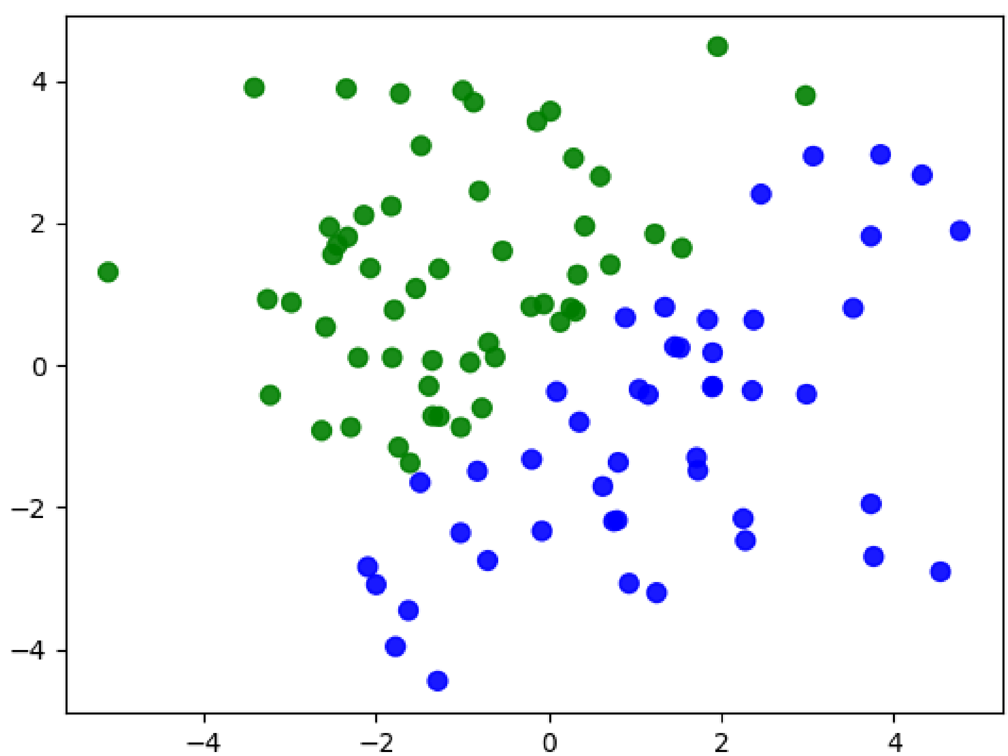
the gradient of which is:

$$\nabla_\beta \mathcal{l}(\mathbf{\beta}) = \frac{1}{N} \sum_{i=1}^{N} x_i (y_i - \sigma(x_i \beta)) $$

d) Plot the loss as a function of b.

In [21]:
```python
%matplotlib widget
from mpl_toolkits import mplot3d
import numpy as np
import matplotlib.pyplot as plt
import sklearn.datasets as datasets

centers = [[0, 0]]
t, _ = datasets.make_blobs(n_samples=100, centers=centers, cluster_std=2

# LINE
def generate_line_data():
    # create some space between the classes
    X = t
    Y = np.array([1 if x[0] - x[1] >= 0 else 0 for x in X])
    return X, Y

X, y = generate_line_data()

cs = np.array([x for x in 'gb'])
fig, ax = plt.subplots()
ax.scatter(X[:, 0], X[:, 1], color=cs[y].tolist(), s=50, alpha=0.9)
plt.show()
```

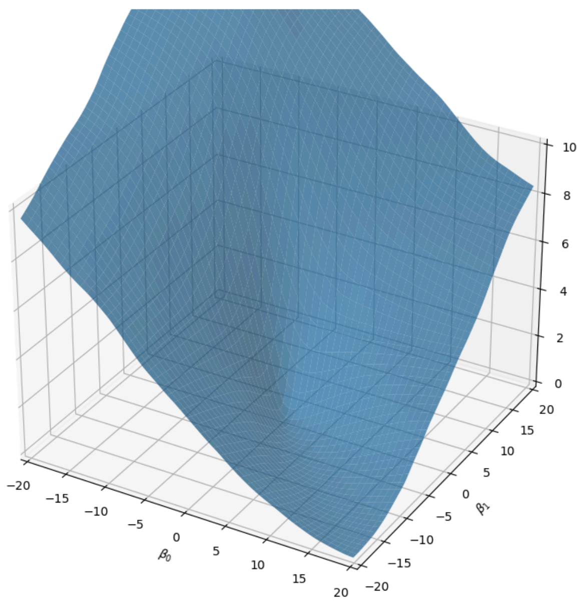
Figure



In [23]:

```
b0 = np.arange(-20, 20, 0.1)
b1 = np.arange(-20, 20, 0.1)
b0, b1 = np.meshgrid(b0, b1)


def sigmoid(x):
    e = np.exp(x)
    return e / (1 + e)


def loss(X, y, beta):
    prob = sigmoid(X @ beta)
    epsilon = 1e-9
    return -np.mean(y * np.log(prob+epsilon) + (1-y) * np.log(1-prob+eps


def get_cost(B0, B1):
    res = []
    for b0, b1 in zip(B0, B1):
        line = []
        for i in range(len(b0)):
            beta = np.array([b0[i], b1[i]])
            line.append(loss(X, y, beta))
        res.append(line)
    return np.array(res)

cost = get_cost(b0, b1)

# Creating figure
fig = plt.figure(figsize =(14, 9))
ax = plt.axes(projection ='3d')
ax.set_xlim(-20, 20)
ax.set_xlabel(r'$\beta_0$')
ax.set_ylabel(r'$\beta_1$')
ax.set_ylim(-20, 20)
ax.set_zlim(0, 10)

# Creating plot
ax.plot_surface(b0, b1, cost, alpha=.7)

# show plot
plt.show()
```

Figure



e) Plot the loss at each iteration of the gradient descent algorithm.

In [24]:

```
import numpy as np
from PIL import Image as im
import matplotlib.pyplot as plt


TEMPFILE = "temp.png"


def snap(betas, losses):
    # Creating figure
    fig = plt.figure(figsize=(14, 9))
    ax = plt.axes(projection='3d')
    ax.view_init(10, 10)
    ax.set_xlabel(r'$\beta_0$')
    ax.set_ylabel(r'$\beta_1$')
    ax.set_ylim(-20, 20)
    ax.set_zlim(0, 10)

    # Creating plot
    ax.plot_surface(b0, b1, cost, color='b', alpha=.7)
    ax.plot(np.array(betas)[:,0], np.array(betas)[:,1], losses, 'o-', c=
    fig.savefig(TEMPFILE)
    plt.close()
    return im.fromarray(np.asarray(im.open(TEMPFILE)))


def gradient(X, y, beta):
    prob = sigmoid(X @ beta)
    return -X.T @ (y-prob) / len(y)


def gradient_descent(X, y, beta_hat, learning_rate, epochs, images):
    losses = [loss(X, y, beta_hat)]
    betas = [beta_hat]

    for _ in range(epochs):
        images.append(snap(betas, losses))
        beta_hat = beta_hat - learning_rate * gradient(X, y, beta_hat)

        losses.append(loss(X, y, beta_hat))
        betas.append(beta_hat)

    return np.array(betas), np.array(losses)


beta_start = np.array([-5, -2])
learning_rate = 0.1
images = []
betas, losses = gradient_descent(X, y, beta_start, learning_rate, 10, ima

images[0].save(
    'gd_logit.gif',
    optimize=False,
    save_all=True,
    append_images=images[1:],
    loop=0,
    duration=500
```

```
)
```

f) Create an animation of the logistic regression fit at every epoch.

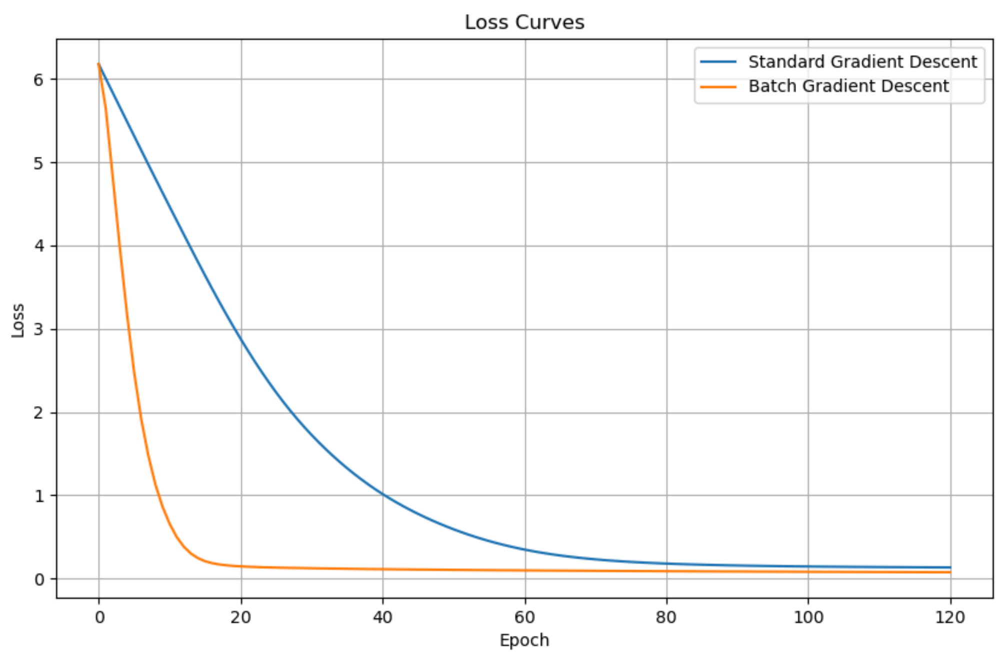
In [25]:
```
def snap_model(beta):
    xplot = np.linspace(-10, 10, 50)
    yestplot = beta[1] + beta[0] * xplot
    fig, ax = plt.subplots()
    ax.plot(xplot, yestplot, 'b-', lw=2)
    ax.scatter(X[:, 0], X[:, 1], color=cs[y].tolist())
    ax.set_xlim(-5, 5)
    ax.set_ylim(-5, 5)
    fig.savefig(TEMPFILE)
    plt.close()
    return im.fromarray(np.asarray(im.open(TEMPFILE)))

def gradient_descent(X, y, beta_hat, learning_rate, epochs, images):
    losses = [loss(X, y, beta_hat)]
    betas = [beta_hat]

    for _ in range(epochs):
        images.append(snap_model(beta_hat))

        beta_hat = beta_hat - learning_rate * gradient(X, y, beta_hat)

        losses.append(loss(X, y, beta_hat))
        betas.append(beta_hat)

    return np.array(betas), np.array(losses)

images = []
betas, losses = gradient_descent(X, y, beta_start, learning_rate, 120, i

images[0].save(
    'model_logit.gif',
    optimize=False,
    save_all=True,
    append_images=images[1:],
    loop=0,
    duration=200
)
```

g) Modify the above code to evaluate the gradient on a random batch of the data. Overlay the true loss curve and the approximation of the loss in your animation.

In [26]:
```python
def gradient_descent(X, y, beta_hat, learning_rate, epochs, images):
    losses = [loss(X, y, beta_hat)]
    betas = [beta_hat]

    for _ in range(epochs):
        images.append(snap_model(beta_hat))

        beta_hat = beta_hat - learning_rate * gradient(X, y, beta_hat)

        losses.append(loss(X, y, beta_hat))
        betas.append(beta_hat)

    return np.array(betas), np.array(losses)


def batch_gradient_descent(X, y, beta_hat, learning_rate, epochs, batch_s
    n_samples = len(y)
    losses = [loss(X, y, beta_hat)]
    betas = [beta_hat]

    for _ in range(epochs):
        images.append(snap_model(beta_hat))

        permuted_indices = np.random.permutation(n_samples)
        batch_losses = []

        for i in range(0, n_samples, batch_size):
            batch_indices = permuted_indices[i:i+batch_size]
            X_batch = X[batch_indices]
            y_batch = y[batch_indices]

            beta_hat = beta_hat - learning_rate * gradient(X_batch, y_ba
            batch_losses.append(loss(X_batch, y_batch, beta_hat))

        losses.append(np.mean(batch_losses))
        betas.append(beta_hat)

    return np.array(betas), np.array(losses)


beta_start = np.array([-5, -2])
learning_rate = 0.1
epochs = 120
batch_size = 20
images = []
b_images = []
betas, losses = gradient_descent(X, y, beta_start, learning_rate, epochs
b_betas, b_losses = batch_gradient_descent(X, y, beta_start, learning_ra

b_images[0].save(
    'model_logit_batch.gif',
    optimize=False,
    save_all=True,
    append_images=b_images[1:],
    loop=0,
    duration=200
)
```

```
plt.figure(figsize=(10, 6))
plt.plot(range(epochs+1), losses, label='Standard Gradient Descent')
plt.plot(range(epochs+1), b_losses, label='Batch Gradient Descent')
plt.title('Loss Curves')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.grid(True)
plt.show()
```

Figure



h) Below is a sandox where you can get intuition about how to tune gradient descent parameters:

In [ ]:

```
import numpy as np
from PIL import Image as im
import matplotlib.pyplot as plt

TEMPFILE = "temp.png"

def snap(x, y, pts, losses, grad):
    fig = plt.figure(figsize =(14, 9))
    ax = plt.axes(projection ='3d')
    ax.view_init(20, -20)
    ax.plot_surface(x, y, loss(np.array([x, y])), color='r', alpha=.4)
    ax.plot(np.array(pts)[:,0], np.array(pts)[:,1], losses, 'o-', c='b',
    ax.plot(np.array(pts)[-1,0], np.array(pts)[-1,1], -1, 'o-', c='b', a

    # Plot Gradient Vector
    X, Y, Z = [pts[-1][0]], [pts[-1][1]], [-1]
    U, V, W = [-grad[0]], [-grad[1]], [0]
    ax.quiver(X, Y, Z, U, V, W, color='g')
    fig.savefig(TEMPFILE)
    plt.close()
    return im.fromarray(np.asarray(im.open(TEMPFILE)))

def loss(x):
    return np.sin(sum(x**2)) # change this

def gradient(x):
    return 2 * x * np.cos(sum(x**2)) # change this

def gradient_descent(x, y, init, learning_rate, epochs):
    images, losses, pts = [], [loss(init)], [init]
    for _ in range(epochs):
        grad = gradient(init)
        images.append(snap(x, y, pts, losses, grad))
        init = init - learning_rate * grad
        losses.append(loss(init))
        pts.append(init)
    return images

init = np.array([-.5, -.5]) # change this
learning_rate = 1.394 # change this
x, y = np.meshgrid(np.arange(-2, 2, 0.1), np.arange(-2, 2, 0.1)) # chang
images = gradient_descent(x, y, init, learning_rate, 12)

images[0].save(
    'gradient_descent.gif',
    optimize=False,
    save_all=True,
    append_images=images[1:],
    loop=0,
    duration=500
)
```