Logistic Regression

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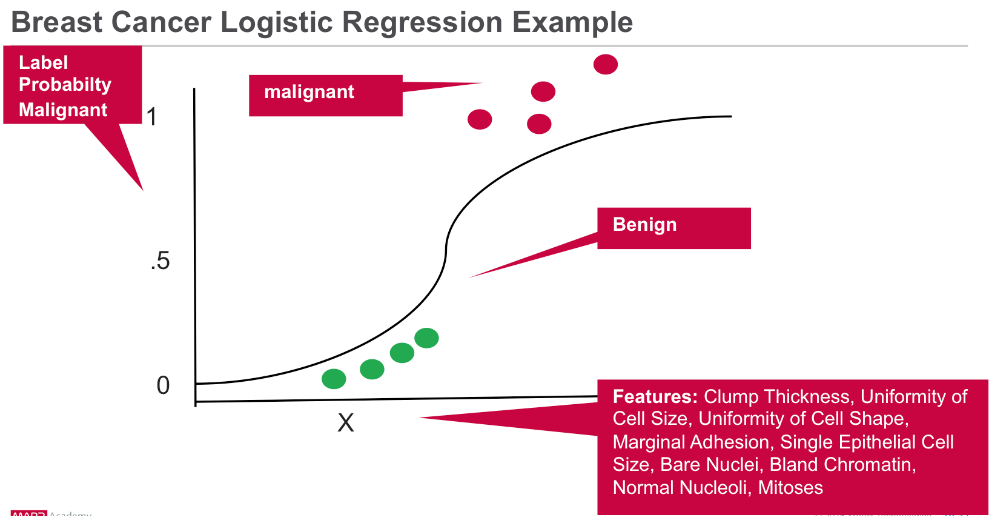
Overview

How do we predict whether an email is spam or not, or if a patient has a disease based on their symptoms? These are classification problems, and logistic regression is a powerful tool for solving them.



Logistic regression predicts probabilities for binary outcomes. It uses the **logistic (sigmoid) function** to model the likelihood of a data point belonging to a particular class.

To optimize the model parameters, we use:

1. **Gradient Descent:** An iterative approach to minimize the cost function.
2. **Newton's Method:** A second-order optimization technique for faster convergence.

In this document, we'll dive into the both methods and their applications.

1. Logistic Regression & Gradient Descent

Logistic regression is a classification algorithm that models the probability of a binary outcome using the logistic (sigmoid) function.

Key Points:

Hypothesis Function: The predicted output (probability) of logistic regression is computed as follows:

- **For a single example:**

$$h_\theta(x^{(i)}) = \frac{1}{1 + e^{-\theta^T x^{(i)}}}$$

Here, $x^{(i)}$ is a single input example.

- **For the entire dataset (input matrix):**

$$h_\theta(X) = \frac{1}{1 + e^{-X\theta}}$$

Where:

  - $x^{(i)}$: A column vector representing the i-th example, containing n features.
    Dimension: $n \times 1$.
  - X: The input matrix containing m examples and n features.
    Dimension: $m \times n$.
  - θ: The parameter vector containing n weights (including θ_0, the bias term).
    Dimension: $n \times 1$.

Cost function:

To optimize θ, we minimize the negative log-likelihood cost function:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \ln(h_\theta(x^{(i)})) + (1 - y^{(i)}) \ln(1 - h_\theta(x^{(i)})) \right]$$

Where:

- m: Number of training examples.
- $y^{(i)}$: Actual label (0 or 1) for the i-th training example.
- $h_\theta(x^{(i)})$: Predicted probability for the i-th training example.

Steps for Batch Gradient Descent of Logistic Regression:

This follows **exactly the same** procedure as Linear Regression. To minimize $J(\theta)$, we compute its gradient and update θ iteratively:

- **Scalar form:**

  For $j = 0, 1, \ldots, n$:

$$\boxed{\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x_j^{(i)}}$$

  Where:

  - $h_\theta(x^{(i)})$ is the predicted output
  - $h_\theta(x^{(i)}) - y^{(i)}$ is the residuals (error compared to actual output)
  - $x_j^{(i)}$ is the j-th feature value of the i-th training example

  Then the parameters θ are updated as:

$$\boxed{\theta_j = \theta_j - \alpha \frac{\partial J(\theta)}{\partial \theta_j}}$$

- **Matrix Form (for all θ):** The gradient can also be written compactly in matrix form as:

$$\boxed{\nabla J(\theta) = \frac{1}{m} X^T (h_\theta(X) - y)}$$

Where:

- X: Feature matrix (including a column of 1s for the bias term).
- $h_\theta(X)$: Vector of predicted probabilities for all training examples.
- y: Vector of actual labels.

Update Rule in Matrix Form:

$$\boxed{\theta = \theta - \alpha \nabla J(\theta)}$$

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2. Newton's Method for Logistic Regression

Newton's method refines the parameters θ using second-order derivative, incorporating the Hessian matrix H:

1. **Gradient:** Same as above:

$$\nabla J(\theta) = \frac{1}{m} X^T (h_\theta(X) - y)$$

2. **Hessian Matrix:**

$$\boxed{H = \frac{1}{m} X^T R X}$$

Where:

- R: Diagonal matrix where $R_{ii} = h_\theta(x^{(i)}) \cdot (1 - h_\theta(x^{(i)}))$.

3. **Update Rule:**

$$\boxed{\theta = \theta - H^{-1} \nabla J(\theta)}$$

Newton's method often converges faster than gradient descent but is computationally expensive for large datasets.

Summary of Key Differences

Aspect	Gradient Descent	Newton's Method
Approach	Iterative, uses first derivative	Iterative, uses first and second derivatives
Computation Cost	Lower per iteration	Higher per iteration due to Hessian inversion
Convergence Speed	Slower for large datasets	Faster, but depends on dataset size
Suitability	Large datasets or high dimensions	Small to medium datasets

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Exercise

Given the training data for a classification problem, to identify if a person is male/female base on his/her weight and high. Stating at $\theta_0 = \theta_1 = \theta_2 = 0$ and learning rate $\alpha = 0.001$.

Training example	Height(cm)	Weight (kg)	Gender
1	172	68	Male
2	163	52	Female
3	158	50	Female
4	180	75	Male

Calculate the coefficients after the first iteration with

a) Batch-gradient descent.

b) Newton method

Part a: Using Batch-gradient descent

In [15]:

```
#Dataset
import numpy as np
X = np.array([
    [1,172,68],
    [1,163,52],
    [1,158,50],
    [1,180,75]
]) #Add a column of 1 to the left to represent the bias term X_0
y = np.array([0,1,1,0]) # 0 for male, 1 for female

m = len(y)
alpha = 0.001
```

In [16]:

```
theta = np.array([0,0,0],dtype=float)
def hypothesis(X, theta):
    return 1 / (1 + np.exp(-X @ theta))

def cost_func(predictions, y):
    return -1/m * np.sum(y*np.log(predictions) + (1-y)*np.log(1-predictions))

iterations = 100
for i in range(1,iterations+1):
    predictions = hypothesis(X,theta)

    errors = predictions - y

    gradient = 1/m * (X.T @ errors)

    theta -= alpha * gradient

    if (i==1):
        print("After the first iteration:")
        print("Predictions: ",predictions)
        print("Errors: ", errors)
        print("Gradient: ",gradient)
        print("Theta = ",theta)
        print("Cost = ",cost_func(predictions,y),"\n")

    if (i%10==0):
        print(f"Iteration {i}: Theta = {theta}, Cost = {cost_func(predictions,y):.4f}
```

```
After the first iteration:
Predictions:  [0.5 0.5 0.5 0.5]
Errors:  [ 0.5 -0.5 -0.5  0.5]
Gradient:  [0.    3.875 5.125]
Theta =  [ 0.       -0.003875 -0.005125]
Cost =  0.6931471805599453

Iteration 10: Theta = [ 0.00038151  0.02552992 -0.0277586 ], Cost = 5.7494
Iteration 20: Theta = [ 0.00068845  0.03880599 -0.05969616], Cost = 5.4982
Iteration 30: Theta = [ 0.0009826   0.05043766 -0.09177184], Cost = 5.3825
Iteration 40: Theta = [ 0.0012791  0.0629325 -0.1231119], Cost = 5.1787
Iteration 50: Theta = [ 0.0015715   0.07509407 -0.15425996], Cost = 4.9968
Iteration 60: Theta = [ 0.0018635   0.08748283 -0.18507323], Cost = 4.7880
Iteration 70: Theta = [ 0.00215382  0.09980324 -0.21573278], Cost = 4.5807
Iteration 80: Theta = [ 0.00244351  0.11218556 -0.24623472], Cost = 4.3643
Iteration 90: Theta = [ 0.00273237  0.12455841 -0.27664243], Cost = 4.1461
Iteration 100: Theta = [ 0.00302071  0.13694618 -0.30696939], Cost = 3.9242
```

In [17]:

```
#Assume me, a guy who is 170cm short and 62kg fat, lets see what gender I am
def what_gender_am_I(height,weight):
    tmd = np.array([1,height,weight])
    tmd_gender = hypothesis(tmd,theta)
    print(tmd_gender)

    if (tmd_gender < 0.5): #male
        print("A dude 🤨")
    elif (tmd_gender > 0.5): #female
        print("A cutie patooie 😍")

what_gender_am_I(170,62)
```

```
0.9859608815891429
A cutie patooie 😍
```

Part b: Using Newton method

Recall:

$$\nabla J(\theta) = \frac{1}{m} X^T (h_\theta(X) - y)$$

$$H = \frac{1}{m} X^T R X$$

$$\theta = \theta - H^{-1} \nabla J(\theta)$$

In [18]:

```
theta = np.array([0,0,0],dtype=float)

def hypothesis(X,theta):
    return 1 / (1+ np.exp(-X @ theta))

def compute_gradient(X,y,theta):
    gradient = 1/m * X.T @ (hypothesis(X,theta) - y)
    return gradient

def compute_hessian(X,theta):
    h = hypothesis(X,theta)
    R = np.diag(h*(1-h))
    return 1/m * (X.T @ R @ X)

gradient = compute_gradient(X, y, theta)
hessian = compute_hessian(X, theta)
```

```python
theta = theta - np.linalg.inv(hessian) @ gradient

print("After one iteration: ")
print("Gradient:\n", gradient)
print("Hessian:\n", hessian)
print("Updated Theta:\n", theta)
```

```
After one iteration:
Gradient:
 [0.    3.875 5.125]
Hessian:
 [[2.5000000e-01 4.2062500e+01 1.5312500e+01]
 [4.2062500e+01 7.0948125e+03 2.5982500e+03]
 [1.5312500e+01 2.5982500e+03 9.6581250e+02]]
Updated Theta:
 [-19.26812373   0.25391138  -0.38289741]
```

In [19]:
```python
#Now let's ask for Mr.Newton's opinion about my gender
what_gender_am_I(170,62)
```

```
0.539212276978382
A cutie patooie 😍
```

In [20]:
```python
#Maybe Mr.Newton will change his mind after 20 iterations?
theta = np.array([0,0,0],dtype=float)
iterations = 20
for i in range(1,iterations+1):
    gradient = compute_gradient(X, y, theta)
    hessian = compute_hessian(X, theta)
    theta = theta - np.linalg.inv(hessian) @ gradient

what_gender_am_I(170,62)
```

```
0.2076754683472401
A dude 🤨
```

BONUS: Tips for your model to work correctly and efficiently:

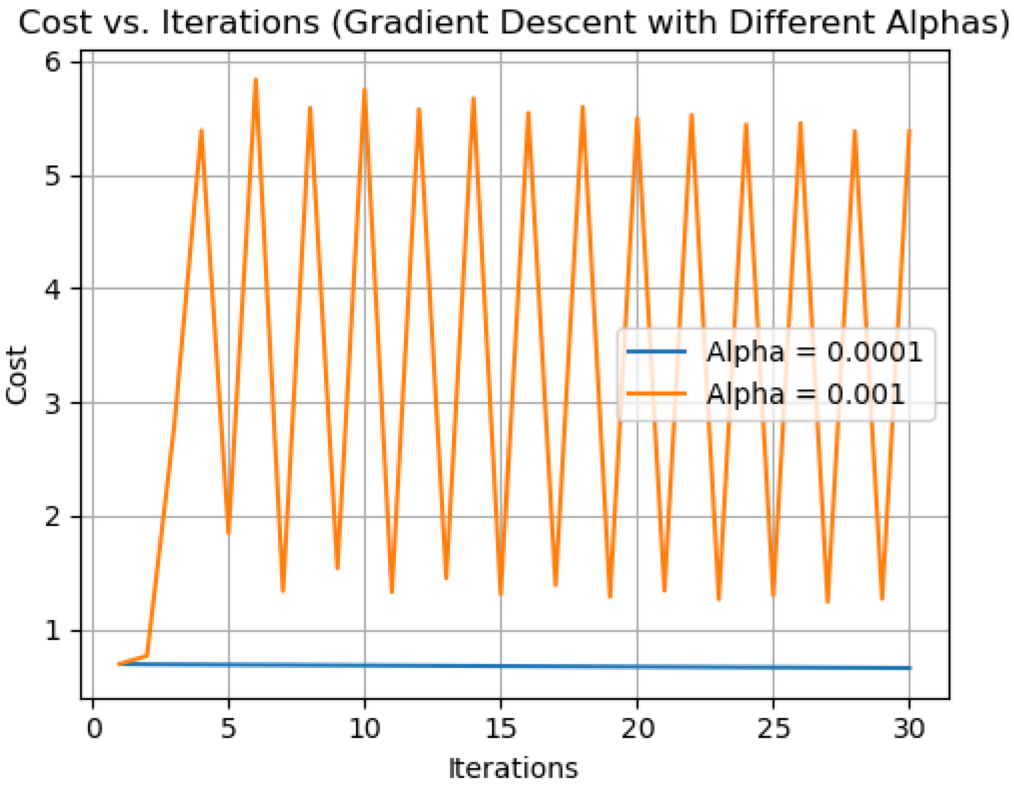
- Try different values of the hyperparameter α, whether it is 0.1, 0.01 or 0.001
- Add more and more iterations so your model can reach the optimal solution
- Try different initial parameters to begin with. A cost function may have many local minimums, yet there is only 1 global minimum.
- Visualize convergence by plotting the cost function over iterations to confirm it is decreasing.

Here's a quick visualization for the Gradient Descent with different values of α

In [21]:
```python
import matplotlib.pyplot as plt
def gradient_descent(X, y, alpha, iterations):
    theta = np.array([0,0,0], dtype=float)
    costs = []

    for i in range(1, iterations + 1):
        predictions = hypothesis(X, theta)
        errors = predictions - y
        gradient = 1/m * (X.T @ errors)
        theta -= alpha * gradient

        cost = cost_func(predictions, y)
```

```python
        costs.append(cost)

        if i == 1 or i % 10 == 0:
            print(f"Alpha = {alpha}, Iteration {i}: Theta = {theta}, Cost = {cost:.4f

    return theta, costs

iterations = 30
alphas = [0.0001, 0.001]
costs_by_alpha = {}

for alpha in alphas:
    print(f"\nRunning gradient descent with alpha = {alpha}...")
    theta, costs = gradient_descent(X, y, alpha, iterations)
    costs_by_alpha[alpha] = costs

plt.figure(figsize=(5.6, 4.2))
for alpha, costs in costs_by_alpha.items():
    plt.plot(range(1, iterations + 1), costs, label=f"Alpha = {alpha}")

plt.xlabel("Iterations")
plt.ylabel("Cost")
plt.title("Cost vs. Iterations (Gradient Descent with Different Alphas)")
plt.legend()
plt.grid()
plt.show()
```

```
Running gradient descent with alpha = 0.0001...
Alpha = 0.0001, Iteration 1: Theta = [ 0.        -0.0003875 -0.0005125], Cost = 0.6931
Alpha = 0.0001, Iteration 10: Theta = [ 2.61383667e-05  5.59458853e-04 -3.47731806e-0
3], Cost = 0.6806
Alpha = 0.0001, Iteration 20: Theta = [ 5.56316431e-05  1.73488809e-03 -6.68271752e-0
3], Cost = 0.6689
Alpha = 0.0001, Iteration 30: Theta = [ 8.47464161e-05  2.89547698e-03 -9.84821154e-0
3], Cost = 0.6575

Running gradient descent with alpha = 0.001...
Alpha = 0.001, Iteration 1: Theta = [ 0.       -0.003875 -0.005125], Cost = 0.6931
Alpha = 0.001, Iteration 10: Theta = [ 0.00038151  0.02552992 -0.0277586 ], Cost = 5.7
494
Alpha = 0.001, Iteration 20: Theta = [ 0.00068845  0.03880599 -0.05969616], Cost = 5.4
982
Alpha = 0.001, Iteration 30: Theta = [ 0.0009826   0.05043766 -0.09177184], Cost = 5.3
825
```



As you can see, with α = 0.0001, our cost steadily decreases while it fluctuates with α = 0.001

This document was created in Jupyter Notebook by Trần Minh Dương (tmd).

If you have any questions or notice any errors, feel free to reach out via Discord at @tmdhoctiengphap or @ICT-Supporters on the USTH Learning Support server.

Check out my GitHub repository for more projects: GalaxyAnnihilator/MachineLearning .