Machine Learning Visualized

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Contents

NumPy citation: [?]

PyTorch citation: [?]

0.1 Gradient Descent

Gradient Descent is an algorithm that finds the local extrema of a function. This is applicable to machine learning, because we want to find the optimal parameters that minimize our loss function. In machine learning, loss functions quantify the amount of error between the predicted values from a machine learning model and the actual expected values. In this notebook, we will perform linear regression by using gradient descent to find the optimal slope and y-intercept.

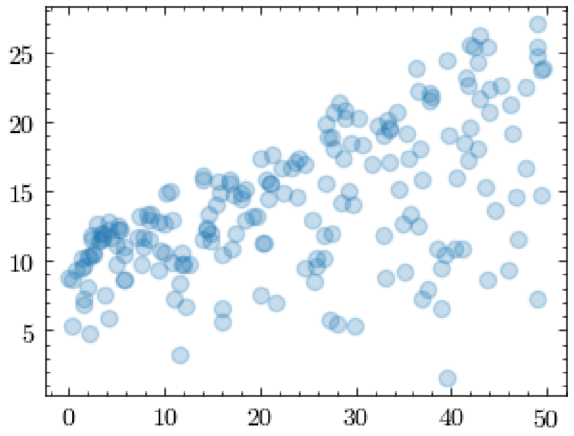
0.1.1 Training Dataset

Importing the libraries

```
import numpy as np

import matplotlib.pyplot as plt
import scienceplots
from IPython.display import display, Latex, Image

from celluloid import Camera

np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

Let's look at the training dataset. We will use columns 2 and 4 of the txt file. The linear regression model will find the optimal slope and y-intercept to fit the data.

```
fname = "REGRESSION-gradientDescent-data.txt"
x, y = np.loadtxt(fname, delimiter=",", unpack=True, skiprows=1, usecols=(2, 4))

fig = plt.figure()
ax = fig.add_subplot()
ax.scatter(x, y, color="#1f77b4", marker="o", alpha=0.25)
```



0.1.2 Loss Function: Mean Squared Error

For the linear regression model, the predicted value $\hat{y}$ is the dot product of the weight and x input vectors plus a bias term

$\hat{y} = wx + b$

We will use the mean squared error function as our loss function.

$$
\begin{aligned}
MSE &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y})^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))^2
\end{aligned}
$$

0.1.3 Loss Function Gradient

```
def mse_loss(x, y, w, b):
    return np.mean(np.square(y - (w * x + b)))
```

In each epoch of gradient descent, a parameter is updated by subtracting the product of the gradient of the function and the learning rate (lr). The learning rate controls how much the parameters should change. Small learning rates are precise, but are slow. Large learning rates are fast, but may prevent the model from finding the local extrema.

$$X_{n+1} = X_n - lr * \frac{\partial}{\partial X} f(X_n)$$

Since we are finding the optimal slope (w) and y-intercept (b) for our linear regression model, we must find the partial derivatives of the loss function with respect to w and b.

0.1.4 Loss Function in Terms of W

Loss function with respect to w:

$$\begin{aligned}
\frac{\partial}{\partial w}(MSE) &= \frac{\partial}{\partial w}[\frac{1}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))^2] \\
&= \frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial w}[(y_i - (wx_i + b))^2] \\
&= \frac{2}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))\frac{\partial}{\partial w}[y_i - (wx_i + b)] \\
&= \frac{2}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))(-x_i) \\
&= -\frac{2}{n}\sum_{i=1}^{n}x_i(y_i - (wx_i + b))
\end{aligned}$$

```
def mse_loss_dw(x, y, w, b):
    return -2 * np.mean(x * (y - (w * x + b)))
```

0.1.5 Loss Function in Terms of b

Loss function with respect to b:

$$
\begin{aligned}
\frac{\partial}{\partial b}(MSE) &= \frac{\partial}{\partial b}[\frac{1}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))^2] \\
&= \frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial b}[(y_i - (wx_i + b))^2] \\
&= \frac{2}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))\frac{\partial}{\partial b}[y_i - (wx_i + b)] \\
&= \frac{2}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))(-1) \\
&= -\frac{2}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))
\end{aligned}
$$

```
def mse_loss_db(x, y, w, b):
    return -2 * np.mean(y - (w * x + b))
```

0.1.6 Training the Linear Regression Model

Let's define a function that uses the gradient algorithm to update the parameters of the loss function. The function uses the gradient functions we derived earlier.

General Gradient Descent Equation:

$$
X_{n+1} = X_n - \mathrm{lr} \cdot \frac{\partial}{\partial X} f(X_n)
$$

Bias Gradient Descent:

$$
\begin{aligned}
b &= b - \eta\frac{\partial}{\partial b}[L(\vec{w}, b)] \\
&= b - \eta[-\frac{2}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))]
\end{aligned}
$$

Weights Gradient Descent:

$$
\begin{aligned}
b &= b - \eta\frac{\partial}{\partial b}[L(\vec{w}, b)] \\
&= b - \eta[-\frac{2}{n}\sum_{i=1}^{n}x_i(y_i - (wx_i + b))]
\end{aligned}
$$

```
def update_w_and_b(x, y, w, b, learning_rate):
    # update w and b
    w = w - mse_loss_dw(x, y, w, b) * learning_rate
    b = b - mse_loss_db(x, y, w, b) * learning_rate

    return w, b
```

0.1.7 Graphing functions

Let's define helper functions to plot the graphs.

```
def create_plots():
    plt.ioff()
    fig = plt.figure(figsize=(16 / 9.0 * 4, 4 * 1), layout="constrained")
    fig.suptitle("Gradient Descent")
    ax0 = fig.add_subplot(1, 2, 1)
    ax0.set_xlabel("Spending", fontweight="normal")
    ax0.set_ylabel("Sales", fontweight="normal")
    ax0.set_title("Linear Regression")

    ax1 = fig.add_subplot(1, 2, 2, projection="3d")
    ax1.set_xlabel("Slope, w")
    ax1.set_ylabel("Intercept, b")
    ax1.set_zlabel("Error")
    ax1.set_title("Error")
    ax1.view_init(15, -35)

    camera = Camera(fig)
    return ax0, ax1, camera


def generate_error_range(x, y, N, w_max, b_max):
    w_range = np.arange(0, w_max, w_max / N)
    b_range = np.arange(0, b_max, b_max / N)
    w_range, b_range = np.meshgrid(w_range, b_range)
    w_range = w_range.flatten()
    b_range = b_range.flatten()

    error_range = np.array([])
    for i in range(min(w_range.shape[0], b_range.shape[0])):
        error_range = np.append(error_range, mse_loss(x, y, w_range[i], b_range[i]))

    return w_range, b_range, error_range
```

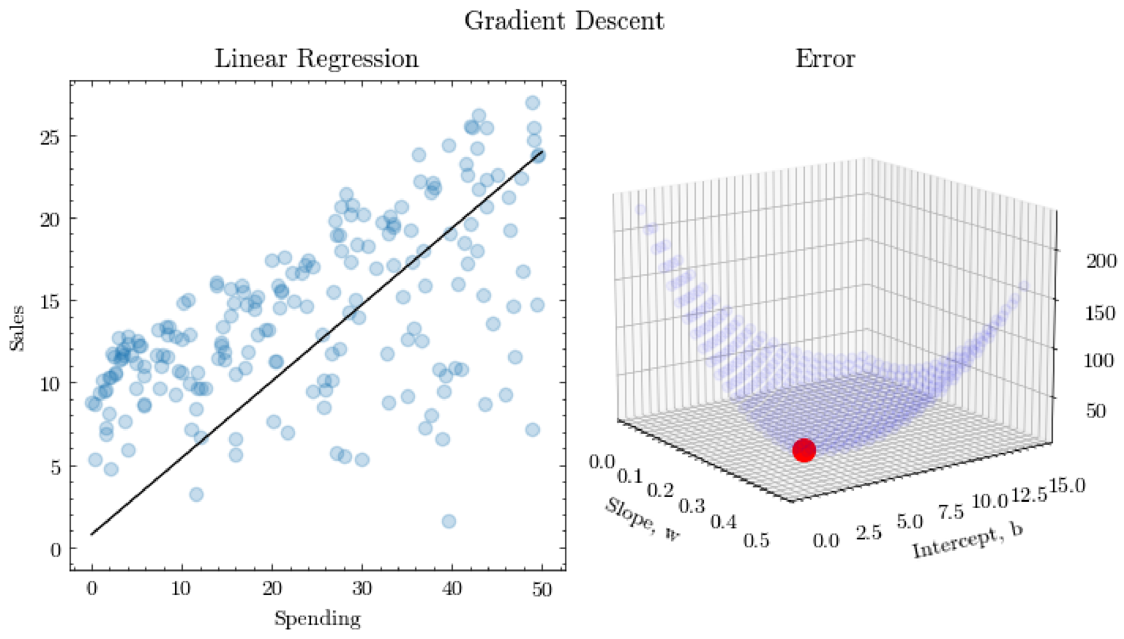
0.1.8 Training the model

The train function will update the parameters in each epoch and update the visualization.

```
def train(x, y, w0, b0, learning_rate, epochs, output_filename):
    w = w0
    b = b0

    ax0, ax1, camera = create_plots()
    loss_dims = 20
    w_max = 0.5
    b_max = 15
    w_range, b_range, error_range = generate_error_range(x, y, loss_dims, w_max, b_max)

    for e in range(epochs):
        w, b = update_w_and_b(x, y, w, b, learning_rate)
        if (
            (e == 0)
            or (e < 60 and e % 5 == 0)
            or (e < 3000 and e % 1000 == 0)
            or (e % 3000 == 0)
        ):
            # Plot the error given the current slope and y-intercept
            ax1.scatter(w_range, b_range, error_range, color="blue", alpha=0.05)
            ax1.scatter([w], [b], [mse_loss(x, y, w, b)], color="red", s=100)

            # Plot the linear regression lines
            ax0.scatter(x, y, color="#1f77b4", marker="o", alpha=0.25)
            X_plot = np.linspace(0, 50, 50)
            ax0.plot(X_plot, X_plot * w + b, color="black")

            # print the loss
            print("epoch: ", str(e), "loss: " + str(mse_loss(x, y, w, b)))
            camera.snap()

    animation = camera.animate()
    animation.save(output_filename, writer="pillow")
    plt.show()

    return w, b
```

Let's train the linear regression model on a sample dataset.

```
fname = "REGRESSION-gradientDescent-data.txt"
x, y = np.loadtxt(fname, delimiter=",", unpack=True, skiprows=1, usecols=(2, 4))
output_filename = "gradient_descent.gif"
train(x, y, 0.0, 0, 0.00005, 4000, output_filename)
```



0.2 K-Means Clustering

This is an unsupervised clustering algorithm that assigns points to a centroid. This is a quick way of grouping data points together and to identify outliers. The downside of this algorithm is that it takes up a lot of memory as everything has to be loaded in. However, it is very easy to implement and has many use cases

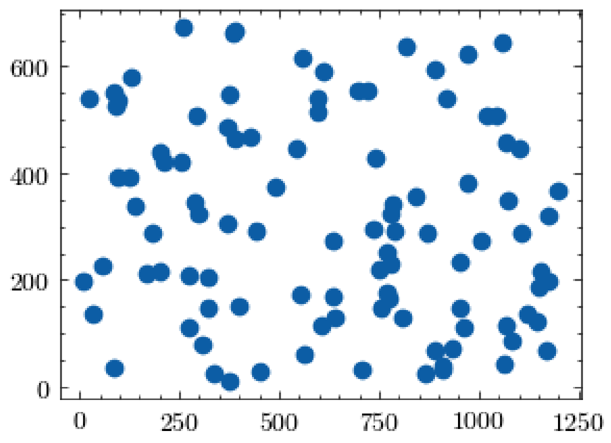
Import the libraries

```
import numpy as np

import matplotlib.pyplot as plt
import scienceplots

from IPython.display import Image
from celluloid import Camera

np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

0.2.1 Example Dataset

Let's generate a dataset of random points

```
K = 12
w = 1200
h = 675
nums = 100

colors = np.random.rand(K, 3)

x = np.random.randint(0, w, size=nums)
y = np.random.randint(0, h, size=nums)
pts = np.column_stack((x, y))

# plot the points
fig = plt.figure()
ax = fig.add_subplot(111)

ax.scatter(x, y)
```



0.2.2 Distance Functions

When assigning points to centroids, we assign them to the closest centroid. In order to quantify this, we need to state how we measure distance. The following are 2 examples of distance functions.

Given point $p1$ at (x_1, y_1) and point $p2$ at (x_2, y_2), we can develop the following distance functions

Euclidean Distance: $\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$

Manhattan Distance: $|x_2 - x_1| + |y_2 - y_1|$

```
def euclidean_distance(p1, p2):
    return np.sqrt((p1[0] - p2[0]) ** 2 + (p1[1] - p2[1]) ** 2)


def manhattan_distance(p1, p2):
    return abs(p1[0] - p2[0]) + abs(p1[1] - p2[1])
```

0.2.3 K Means Setup

At the beginning, the centroids are initialized with random x and y values.

```
centroids_x = np.random.randint(0, w, size=K)
centroids_y = np.random.randint(0, h, size=K)
centroids = np.column_stack((centroids_x, centroids_y))
```

0.2.4 Graphing Functions

Create a helper function to create a plot with the sum of the distances squared on the left and the centroids on the right. Also initialize variables for the visualization, like the sum of the distances so far.

```
def create_plots():
    fig, ax = plt.subplots(1, 3, figsize=(16 / 9.0 * 4, 4 * 1), layout="constrained")
    fig.suptitle("K-Means Clustering Unsupervised")

    ax[0].set_xlabel("K Clusters", fontweight="normal")
    ax[0].set_ylabel("Sum of Euclidean Distance Squared", fontweight="normal")
    ax[0].set_title("Elbow Method")

    ax[1].axis("off")
    ax[2].axis("off")

    ax[2] = fig.add_subplot(1, 2, 2)
    ax[2].set_xlabel("X")
    ax[2].set_ylabel("Y")
    ax[2].set_title("Centroids")

    camera = Camera(fig)
    return ax[0], ax[2], camera

boundary_div = 25
x_boundary_inc = int(w / boundary_div)
y_boundary_inc = int(h / boundary_div)

x_boundary = np.linspace(0, w, x_boundary_inc + 1)
y_boundary = np.linspace(0, h, y_boundary_inc + 1)
x_boundary, y_boundary = np.meshgrid(x_boundary, y_boundary)
colors_idx_boundary = np.random.randint(0, K, size=x_boundary.shape)

x_boundary_flat = x_boundary.flatten()
y_boundary_flat = y_boundary.flatten()

dists = np.zeros(K)
dists_idx = np.arange(1, K + 1)
```

0.2.5 Training the Model

Let's bring everything together. In this visualization, I show the centroids with varying values of K, which is the total number of centroids. For every value of K, I run the algorithm for a certain number of epochs. At the start, centroids start at a random location on the grid. In each epoch, points are assigned to the closest centroid. Then, the next location of the centroid is the average x and y value of all the points assigned to it in the previoius iteration.

```
ax0, ax1, camera = create_plots()
epochs = 8

output_filename = "k_means.gif"

for k in range(1, K + 1):
    acc_dist_squared = 0
    for e in range(epochs):
        # Draw the boundaries
        for index in np.ndindex(x_boundary.shape):
            x = x_boundary[index]
            y = y_boundary[index]

            colors_idx_boundary[index] = 0
            min_group = 0
            # set min distance to largest possible distance initially
            min_dist = np.sqrt(w**2 + h**2)

            curr_pt = [x, y]
            curr_c = []
            for c in range(k):
                curr_c = centroids[c]

                dist = euclidean_distance(curr_pt, curr_c)
                if dist < min_dist:
                    min_dist = dist
                    min_group = c
            colors_idx_boundary[index] = min_group

        colors_boundary = colors[colors_idx_boundary.flatten()]
        ax1.scatter(
            x_boundary_flat, y_boundary_flat, c=colors_boundary, s=20, alpha=0.45
        )

        # Assign each point to a centroid
        groups = [[] for _ in range(k)]
        acc_dist_squared = 0
        for i in range(nums):
            min_group = 0
            # set min distance to largest possible distance initially
            min_dist = np.sqrt(w**2 + h**2)

            curr_pt = pts[i]
            curr_c = []
            for c in range(k):
                curr_c = centroids[c]

                dist = euclidean_distance(curr_pt, curr_c)
                if dist < min_dist:
                    min_dist = dist
                    min_group = c

            groups[min_group].append(curr_pt)
            acc_dist_squared += min_dist**2

        # Centroids
        for g in range(k):
            # Draw the centroids
            curr_centroid = centroids[g]
            curr_centroid = np.array([curr_centroid], dtype=np.int32)
            ax1.scatter(curr_centroid[:, 0], curr_centroid[:, 1], color=colors[g], s=8)

            group_pts = np.array(groups[g])
            if group_pts.size != 0:
                # Draw lines between points and the centroids
                pts_in_group = group_pts.shape[0]
                for i in range(pts_in_group):
                    group_pt = group_pts[i]
                    ax1.plot(
                        [group_pt[0], centroids[g][0]],
                        [group_pt[1], centroids[g][1]],
                        color=colors[g],
                        linewidth=2,
                        alpha=0.55,
                    )

                # Update the location of the centroids
                new_centroid = np.mean(group_pts, axis=0)
                centroids[g] = new_centroid
                new_centroid = np.array([new_centroid], dtype=np.int32)

        # Draw the points
        ax1.scatter(pts[:, 0], pts[:, 1], c="black", s=15, alpha=0.3)
        # Draw the Elbow Method graph
        if k - 2 > 0:
            ax0.plot(dists_idx[: k - 1], dists[: k - 1], color="red")
        camera.snap()
        # if e % 2 == 0:
        #     camera.snap()
        # else:
        #     ax0.clear()
        #     ax1.clear()

    acc_dist_squared /= nums
    dists[k - 1] = acc_dist_squared
    print(k-1, acc_dist_squared)

animation = camera.animate()
animation.save("k_means.gif", writer="pillow")
plt.close()
```

0.3 Principal Component Analysis

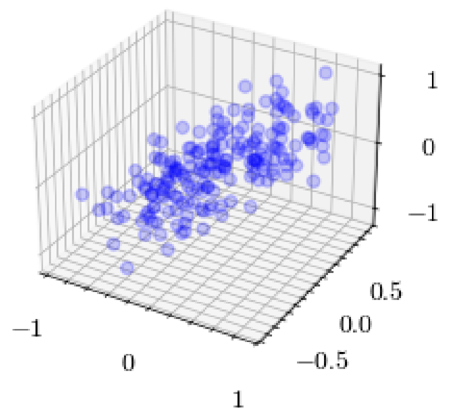
An important decision to make when training machine learning models is the the features to use for the training dataset. Principal Component Analysis allows you to see which features account for most of the variance, simplifying the dataset to a smaller number of correlated variables.

```
import numpy as np

%matplotlib widget
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import scienceplots
from celluloid import Camera

from IPython.display import Image

np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

0.3.1 Target Dataset

Let's generate a noisy list of points by generating points between a start and end point and by adding random noise to each point

```
def generate_noisy_hyperplane(num_points, start_pt, end_pt, noise=0.25):
    # create a plane from the start to the end point
    t = np.linspace(0.0 + noise, 1.0 - noise, num_points).reshape(-1, 1)
    points = start_pt + t * (end_pt - start_pt)

    # add noise to plane
    noise = np.random.normal(0, noise, size=(num_points, 3))
    points = points + noise

    return points


start_pt = np.array([-1, -1, -1])
end_pt = np.array([1, 1, 1])
X = generate_noisy_hyperplane(200, start_pt, end_pt)

# plot the points
fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")
ax.scatter(X[:, 0], X[:, 1], X[:, 2], alpha=0.2, color="blue", label="Original Data")
plt.show()
```



0.3.2 Eigenvectors and Eigenvalues

When you multiply a matrix with its eigenvector, you get a multiple of the eigenvector. The scalar multiple is the eigenvector's eigenvalue. The process of finding the eigenvectors and eigenvalues of a matrix is called Eigendecomposition.

$$A\vec{v} = \lambda\vec{v}$$

The scalar λ is the eigenvalue and the vector $\vec{v}$ is the corresponding eigenvector. The eigendecomposition typically involves solving the determinant $det(A - \lambda I) = 0$, where I is the identity matrix.

Use numpy to quickly get the eigenvalues and eigenvectors of a matrix

```
import numpy as np
mat = np.array([[4, -2],
                [1,  1]])
eig_vals, eig_vecs = np.linalg.eig(mat)
```

0.3.3 Lagrange Multipliers (Optimization with constraints)

Recall from Multivariable Calculus that Lagrange Multipliers allow you to find the extrema of a function $f(x, y, z, ...)$ that is subject to a constraint function $g(x, y, z, ...) = 0$.

The Lagrange Multipliers technique states that the solution of this constrainted optimization problem is the solution to the following system of equations:

$$\nabla L = 0$$

where

$$L(x, y, z, ...\lambda) = f(x, y, z, ...\lambda) - \lambda g(x, y, z, ...\lambda)$$

0.3.4 PCA Derivation (Eigendecomposition of Covariance Matrix)

Recall that our goal is to find the vectors v that account for most of the variance.

Given input vector x_i and vector v, we want to project every input point to v in each dimension.

$$z_i = x_i^T v$$

The variance is

$$(x_i^T v)^2 = z_i^2$$

To find the maximum variance across all of the projections for the n dimensions.

$$\begin{aligned}\max \sum_{i=1}^{n} (x_i^T v)^2 &= \max \sum_{i=1}^{n} z_i^2 \\ &= \max z^T z \\ &= \arg\max (xv)^T xv\end{aligned}$$

Since the ratios of the Principal Components is all that matters, let's introduce the constaint that

$$v^T v = 1$$

Solving the constrainted optimization with Lagrange Multipliers, we define the Lagrangian function:

$$L = \arg\max v^T x^T x v - \lambda(v^T v - 1)$$

Let's solve the Lagrangian function by solving $\nabla L = 0$

$$\begin{aligned}
0 &= \frac{\partial L}{\partial v} \\
&= \frac{\partial}{\partial v}[v^T x^T x v - \lambda(v^T v - 1)] \\
&= 2x^T x v - 2\lambda v \\
&= x^T x v - \lambda v \\
&= (x^T x) v - \lambda v \\
(x^T x) v &= \lambda v
\end{aligned}$$

Given that $x^T x$ is the covariance of a matrix, we see that the solution to PCA is simply the eigendecomposition of the covariance matrix.

0.3.5 PCA Implementation

To recap the two sections above, PCA consists of the following parts: 1. Standard the input data by dividing the difference of the data and the mean by the standard deviation. 2. Compute the covariance matrix of the standardized input 3. Compute eigenvalues and eigenvectors of the covariance matrix 4. To get the projected data, matrix multiply the standardized input and the eigenvectors.

```
def pca(X, dims):
    # subtract the mean to center the data and divide by standard deviation
    X_centered = (X - np.mean(X, axis=0)) / np.std(X, axis=0)

    # compute covariance matrix
    cov = np.cov(X_centered.T)

    # eigendecomposition of the covariance matrix
    # the eigenvectors are the principal components
    # the principal components are the columns of the eig_vecs matrix
    eig_vals, eig_vecs = np.linalg.eig(cov)

    # sort the eigenvalues and eigenvectors
    sorted_idx = np.argsort(eig_vals)[::-1]
    eig_vals = eig_vals[sorted_idx]
    eig_vecs = eig_vecs[:, sorted_idx]

    # perform dimensionality reduction using the computed principal components
    # if you want to reduce to K dimensions, simplify take the first K columns
    projected = X_centered @ eig_vecs

    # compute the variance of each dimension (column)
    pc_variances = [np.var(projected[:, i]) for i in range(dims)]

    return eig_vals, eig_vecs, projected, pc_variances
```

0.3.6 Graphing Functions

Utility functions to create the visualizations

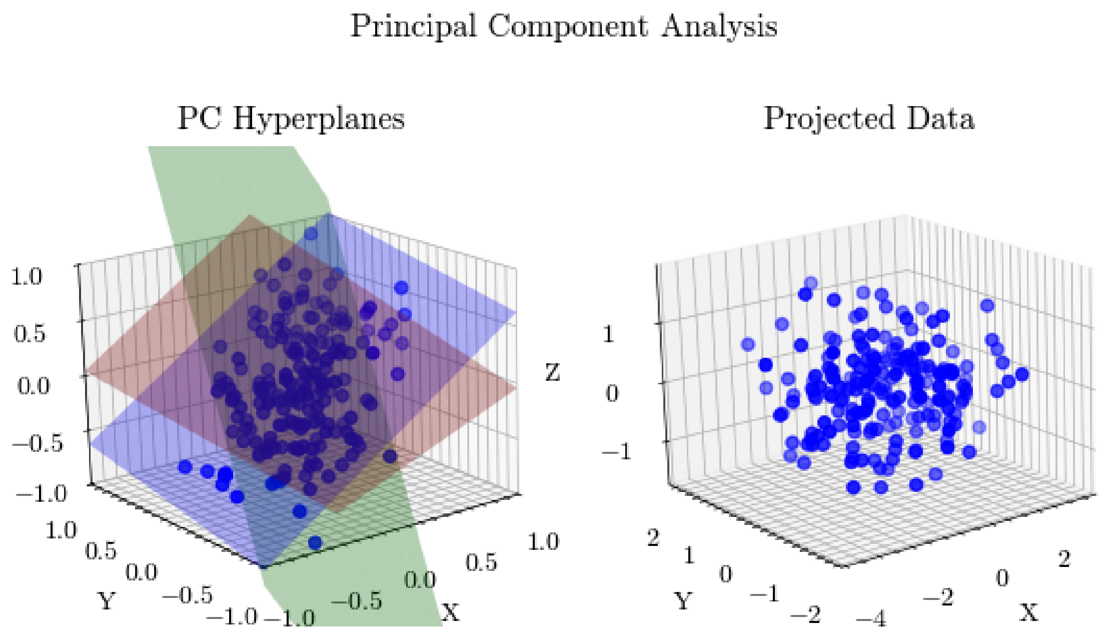
```python
def create_plots():
    fig = plt.figure(figsize=(16 / 9.0 * 4, 4 * 1))
    fig.suptitle("Principal Component Analysis")

    ax0 = fig.add_subplot(121, projection="3d")
    ax0.set_xlabel("X")
    ax0.set_ylabel("Y")
    ax0.set_zlabel("Z")
    ax0.set_title("PC Hyperplanes")
    ax0.view_init(17, -125, 2)
    ax0.set_xlim(-1, 1)
    ax0.set_ylim(-1, 1)
    ax0.set_zlim(-1, 1)
    ax0.tick_params(axis="both", which="both", length=0)

    ax1 = fig.add_subplot(122, projection="3d")
    ax1.set_xlabel("X")
    ax1.set_ylabel("Y")
    ax1.set_zlabel("Z")
    ax1.set_title("Projected Data")
    ax1.view_init(17, -125, 2)
    # ax1.set_xlim(-1, 1)
    # ax1.set_ylim(-1, 1)
    # ax1.set_zlim(-1, 1)
    ax1.tick_params(axis="both", which="both", length=0)
    # plt.axis('equal')

    camera = Camera(fig)
    return ax0, ax1, camera


def plot_hyperplane(ax, pc_vector, color="red", scaling=10, alpha=0.3):
    # Create a grid of points
    points = np.linspace(-1, 1, scaling)
    xx, yy = np.meshgrid(points, points)

    # the z value is the defined by the hyperplane from the principal component vector
    pc_vector /= np.linalg.norm(pc_vector)
    z = (-pc_vector[0] * xx - pc_vector[1] * yy) / pc_vector[2]

    ax.plot_surface(xx, yy, z, color=color, alpha=alpha)
```

0.3.7 Visualize PCA

Given the derivation of PCA, let's visualize the projected data with different values for the target dimension.

```python
def visualize_pca(X, dims, output_filename):
    ax0, ax1, camera = create_plots()
    colors = ["red", "green", "blue"]

    for dim in range(0, dims + 1):
        eig_vals, eig_vecs, projected, pc_variances = pca(X, dims)

        # plot the original data
        ax0.scatter(X[:, 0], X[:, 1], X[:, 2], color="blue", label="Original Data")

        # plot the pca hyperplanes
        for i in range(dim):
            plot_hyperplane(ax0, eig_vecs[:, i], color=colors[i])

        # plot the projected data from the principal components
        curr_projected = projected
        for i in range(dim, dims):
            if i < dims:
                curr_projected[:, i] = 0
        if dim != 0:
            ax1.scatter(
                curr_projected[:, 0],
                curr_projected[:, 1],
                curr_projected[:, 2],
                color="blue",
                label="Projected Data",
            )

        camera.snap()

    animation = camera.animate(interval=2000)
    animation.save(output_filename, writer="pillow")
    plt.show()

    eig_vals, eig_vecs, projected, pc_variances = pca(X, dims)

    print("variance percentage per principal component")
    variance_percentage = eig_vals / np.sum(eig_vals)
    for i, percentage in enumerate(variance_percentage):
        print(f"{i+1}th PC: {round(percentage*100, 2)}%")

    print("variance per principal component")
    for i, variance in enumerate(pc_variances):
        print(f"{i+1}th PC: {round(variance, 2)}")

    print("\nhyperplanes")
    for i in range(dim):
        print(f"hyperplane {i}: {eig_vecs[:, i]}")
```

```
dims = 3
output_filename = "pca.gif"

visualize_pca(X, dims, output_filename)
```



0.3.8 Scikit-Learn Implementation

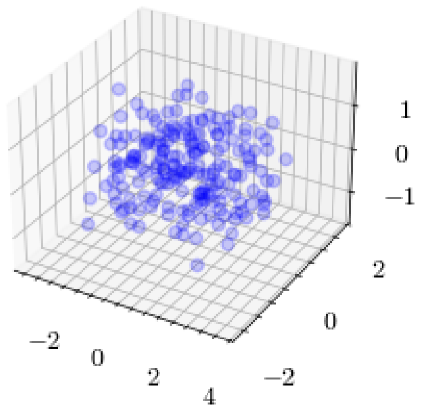
As a check for correctness, let's compare our results with the PCA module from scikit-learn.

Note: The sign of the values might not match exactly. They just need to have the same ratios, which they do. Our implementation matches the one from scikit-learn.

```
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
X_centered = scaler.fit_transform(X)

pca = PCA(n_components=dims)
projected = pca.fit_transform(X_centered)
eig_vecs = pca.components_

print("\nhyperplanes")
for i in range(dims):
    print(f"hyperplane {i}: {eig_vecs[i]}")
```

Let's also plot scikit's learn projected data. Our implementation seems to match for the projected as well.

```
fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")
ax.scatter(projected[:, 0], projected[:, 1], projected[:, 2], alpha=0.2, color="blue", label="Projected Data")
plt.show()
```



0.4 Logistic Regression

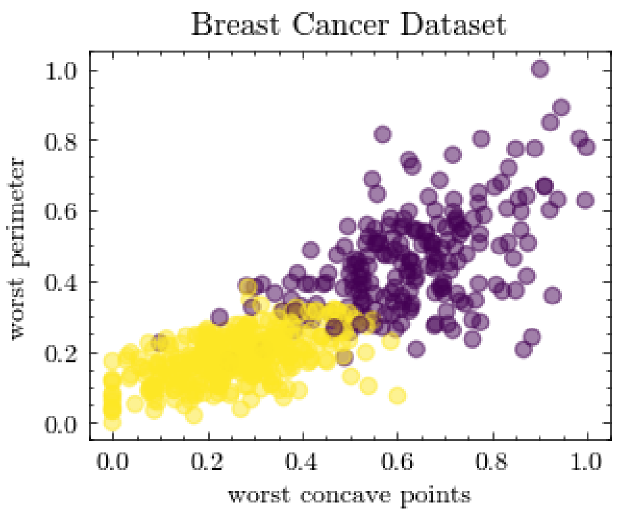
Binary Classification model that finds the optimal the weights and bias and returns probabilites of the two classes

```
# import numpy as np
import autograd.numpy as np
from autograd import grad
from autograd import elementwise_grad as egrad

%matplotlib widget
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

import sklearn.datasets as skdatasets

from celluloid import Camera
import scienceplots
from IPython.display import Image

np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

0.4.1 Training Dataset

Let's import the breast cancer dataset. The logistic regression will perform binary classification using the mean perimeter and mean radius of the tumor.

```
dataset = skdatasets.load_breast_cancer()

features_used = [-3, -8]
X = dataset.data[:, features_used]
feature_names = dataset.feature_names[features_used]

# min-max normalize the features along the columns
X_min_vals = X.min(axis=0)
X_max_vals = X.max(axis=0)
X = (X - X_min_vals) / (X_max_vals - X_min_vals)

Y = dataset.target
target_names = dataset.target_names

fig = plt.figure()
ax = fig.add_subplot()

ax.scatter(X[:, 0], X[:, 1], c=Y, alpha=0.5)
ax.set_xlabel(feature_names[0])
ax.set_ylabel(feature_names[1])
ax.set_title("Breast Cancer Dataset")
```



0.4.2 Activation Function

Recall that the output of the perceptron was the dot product between the weight vector $\vec{w}$ and the input vector $\vec{x}$ plus a constant bias term b

Perceptron: $y = w^T x + b$

Activation functions are applied after the computation.

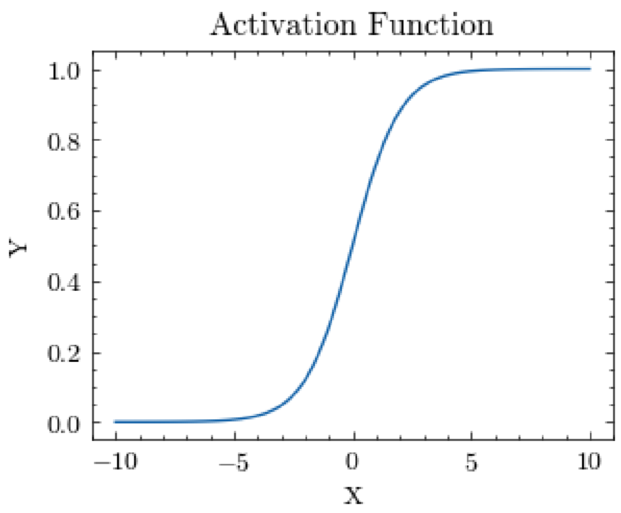
Sigmoid Function

In order to do binary classification, we would like to limit the value of the output to be in the range (0, 1) and get a value to represent the probability of the output being assigned to either class. The sigmoid function is perfect for this

$$\sigma(z) = \frac{1}{1 + e^- z}$$

```
sigmoid = lambda x: 1 / (1 + np.exp(-x))
```

```
def plot(fx, x_min, x_max, points=100, title=""):

    x = np.linspace(x_min, x_max, points)
    y = fx(x)

    fig, axes = plt.subplots()
    axes.plot(x, y)
    axes.set_xlabel("X")
    axes.set_ylabel("Y")
    axes.set_title("Activation Function")


x_min = -10
x_max = 10
points = 100
plot(sigmoid, x_min, x_max, points)
```

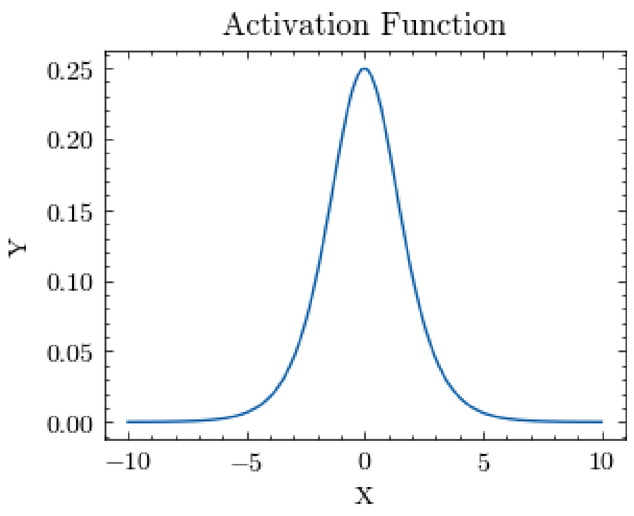


0.4.3 Gradient of Sigmoid Function

Gradient Descent will be used later to find the optimal weight values. As a result, let's calculate the gradient of the sigmoid function.

$$\begin{aligned}
\sigma' &= \frac{\partial}{\partial z}\sigma(z) \\
&= \frac{\partial}{\partial z}(\frac{1}{1+e^{-z}}) \\
&= \frac{\partial}{\partial z}(1+e^{-z})^{-1}) \\
&= (-1)(1+e^{-z})^{-2}\frac{\partial}{\partial z}(1+e^{-z}) \\
&= (-1)(1+e^{-z})^{-2}(e^{-z})\frac{\partial}{\partial z}(-z) \\
&= (-1)(1+e^{-z})^{-2}(e^{-z})(-1) \\
&= \frac{e^{-z}}{(1+e^{-z})^2}
\end{aligned}$$

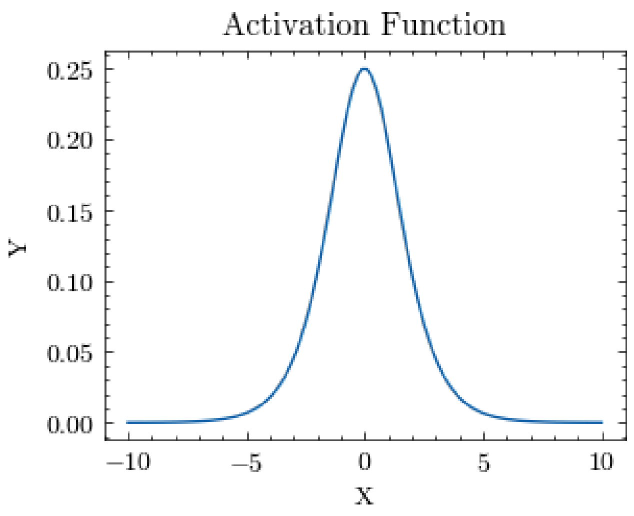
```
sigmoid_prime = lambda x: np.exp(-x) / np.power((1 + np.exp(-x)), 2)
plot(sigmoid_prime, x_min, x_max, points)
```



0.4.4 Autograd

Alternatively, you can use autograd to differentiate a numpy function. Pytorch and JAX also implement autograd.

```
# grad() differentiates scalar inputs
sigmoid_prime_grad = grad(sigmoid)
# egrad() differentiates vectorized inputs
sigmoid_prime_egrad = egrad(sigmoid)

x = np.linspace(x_min, x_max, points)
assert sigmoid_prime_grad(x[0]) == sigmoid_prime(x[0])
assert np.allclose(sigmoid_prime_egrad(x), sigmoid_prime(x))

plot(sigmoid_prime_egrad, x_min, x_max, points)
```



0.4.5 Loss Function

The binary cross entropy loss function will be used for logistic regression. This loss function is derived from the definition of maximum likelihood estimation.

For the binary classification model, the probability of seeing the first class is the sigmoid activation function is applied over the sum of the bias b and the dot product of the weight vector $\vec{w}$ and the input vector $\vec{x}$. The probability of seeing the other class is the difference between 1 and the probability of seeing the other class.

$$P(Y = 1 \mid \vec{x}; \vec{w}, b) = \sigma(\vec{w} \cdot \vec{x} + b)$$

$$P(Y = 0 \mid \vec{x}; \vec{w}, b) = 1 - P(Y = 1 \mid \vec{x}; \vec{w}, b)$$

Maximum Likelihood Estimation

Maximum likelihhod estimation finds the optimal weights and bias to maximize the probability of seeing the training data.

The probability of getting the correct binary prediction function in terms of $\vec{w}$ and b is the following. This can also be thought of as a Bernoulli distribution.

$$P(Y \mid \vec{x}; \vec{w}, b) = [\sigma(\vec{w} \cdot \vec{x} + b)]^{y} \ [1 - \sigma(\vec{w} \cdot \vec{x} + b)]^{1-y}$$

With a training dataset of i examples of $\vec{x_i}$ features and y_i labels, so the total probability is written as the product of the probabilites of all the training examples. Consider this as the likelihood of the training dataset with the current weights and bias.

$$P(Y \mid \vec{x_i}; \vec{w}, b) = \prod_{i=1}^{n} [\sigma(\vec{w} \cdot \vec{x_i} + b)]^{y_i} \ [1 - \sigma(\vec{w} \cdot \vec{x_i} + b)]^{1-y_i}$$

Keep in mind that we want to find the set of optimal parameters $\vec{w}$ and b that maximize the total likelihood.

$$P(Y \mid \vec{x_i}; \vec{w}, b) = \max_{\vec{w}, b} \prod_{i=1}^{n} [\sigma(\vec{w} \cdot \vec{x_i} + b)]^{y_i} \ [1 - \sigma(\vec{w} \cdot \vec{x_i} + b)]^{1-y_i}$$

In order to find the optimal weights and bias for the logistic regression model, we use gradient descent, which is a solution to optimization problems. We have to take the partial derivative of the likelihood with respect to $\vec{w}$ and b.

In it's current form, the total probability is a lot of multiplications. Per the product rule for derivatives, the partial derivatives will also be a lot of multiplication. In order to avoid this, we can take the logarithm of the likelihood, which converts the multiplications into additions.

$$
\begin{aligned}
\ln(P(Y \mid \vec{x_i}; \vec{w}, b)) &= \max_{\vec{w},b} \ln(\prod_{i=1}^{n}[\sigma(\vec{w}\cdot\vec{x_i}+b)]^{y_i}[1-\sigma(\vec{w}\cdot\vec{x_i}+b)]^{1-y_i}) \\
&= \max_{\vec{w},b} \sum_{i=1}^{n}[\ln([\sigma(\vec{w}\cdot\vec{x_i}+b)]^{y_i}[1-\sigma(\vec{w}\cdot\vec{x_i}+b)]^{1-y_i})] \\
&= \max_{\vec{w},b} \sum_{i=1}^{n}[\ln([\sigma(\vec{w}\cdot\vec{x_i}+b)]^{y_i}) + \ln([1-\sigma(\vec{w}\cdot\vec{x_i}+b)]^{1-y_i})] \\
&= \max_{\vec{w},b} \sum_{i=1}^{n}[y_i \ln(\sigma(\vec{w}\cdot\vec{x_i}+b)) + (1-y_i)\ln(1-\sigma(\vec{w}\cdot\vec{x_i}+b))]
\end{aligned}
$$

We define the negative (multiply equation above by -1) log of the likelihood as the binary cross entropy loss function. Let's also divide by the number of training examples to make this the average loss across the n examples.

$$L(\vec{w}, b) = -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(\sigma(\vec{w}\cdot\vec{x_i}+b)) + (1-y_i)\ln(1-\sigma(\vec{w}\cdot\vec{x_i}+b))]$$

Binary Cross Entropy Loss Function

Recall that $\hat{y} = \sigma(\vec{w}\cdot\vec{x}+b) = \frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}}$

To simplify the calculation of the loss, let's rewrite it in terms of $\hat{y}$

$$L(\hat{y}) = -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(\hat{y}_i) + (1-y_i)\ln(1-\hat{y}_i)]$$

```
def bce(y_true, y_pred):
    return -np.sum(y_true * np.log(y_pred) + (1 - y_true) * np.log(1 - y_pred))
```

0.4.6 Loss Function in Terms of W and B

Before taking the partial derivative of the loss function with respect to $\vec{w}$ and b. Let's simplify it to make the partial derivative calculaton easier.

$\hat{y} = \sigma(\vec{w}\cdot\vec{x}+b) = \frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}}$

$$\begin{aligned}
L(\vec{w}, b) &= -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(\sigma(\vec{w}\cdot\vec{x_i}+b)) + (1-y_i)\ln(1-\sigma(\vec{w}\cdot\vec{x_i}+b))] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(\sigma(\vec{w}\cdot\vec{x_i}+b)) - y_i\ln(1-\sigma(\vec{w}\cdot\vec{x_i}+b)) + \ln(1-\sigma(\vec{w}\cdot\vec{x_i}+b))] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(\frac{\sigma(\vec{w}\cdot\vec{x_i}+b)}{1-\sigma(\vec{w}\cdot\vec{x_i}+b)}) + \ln(1-\sigma(\vec{w}\cdot\vec{x_i}+b))] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(\frac{\frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}}}{1-\frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}}}) + \ln(1-\frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}})] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln(e^{\vec{w}\cdot\vec{x_i}+b}) + \ln(\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i(\vec{w}\cdot\vec{x_i}+b) - \ln(1+e^{\vec{w}\cdot\vec{x_i}+b})]
\end{aligned}$$

0.4.7 Loss Function Gradient

Loss function with respect to W

$$\begin{aligned}
\nabla_W[L(\vec{w}, b)] &= \nabla_W[-\frac{1}{n}\sum_{i=1}^{n}[y_i(\vec{w}\cdot\vec{x_i}+b) - \ln(1+e^{\vec{w}\cdot\vec{x_i}+b})]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i\nabla_W[\vec{w}\cdot\vec{x_i}+b] - \nabla_W[\ln(1+e^{\vec{w}\cdot\vec{x_i}+b})]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i x_i - (\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})\nabla_W[1+e^{\vec{w}\cdot\vec{x_i}+b}]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i x_i - (\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})(e^{\vec{w}\cdot\vec{x_i}+b})\nabla_W[\vec{w}\cdot\vec{x_i}+b]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i x_i - (\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})(e^{\vec{w}\cdot\vec{x_i}+b})(x_i)] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i x_i - x_i(\frac{e^{\vec{w}\cdot\vec{x_i}+b}}{1+e^{\vec{w}\cdot\vec{x_i}+b}})] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i x_i - x_i(\frac{1}{1+e^{-(\vec{w}\cdot\vec{x_i}+b)}})] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i x_i - x_i\hat{y}_i] \\
&= \frac{1}{n}\sum_{i=1}^{n}[\hat{y}_i x_i - y_i x_i] \\
&= \frac{1}{n}\sum_{i=1}^{n}[x_i(\hat{y}_i - y_i)]
\end{aligned}$$

```
def bce_dw(x, y_true, y_pred):
    return np.mean(x * (y_pred - y_true))
```

Loss function with respect to b

$$\begin{aligned}
\frac{\partial}{\partial b}[L(\vec{w},b)] &= \frac{\partial}{\partial b}[-\frac{1}{n}\sum_{i=1}^{n}[y_i(\vec{w}\cdot\vec{x_i}+b)-\ln(1+e^{\vec{w}\cdot\vec{x_i}+b})]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i\frac{\partial}{\partial b}[\vec{w}\cdot\vec{x_i}+b]-\frac{\partial}{\partial b}[\ln(1+e^{\vec{w}\cdot\vec{x_i}+b})]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i(1)-(\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})\frac{\partial}{\partial b}[1+e^{\vec{w}\cdot\vec{x_i}+b}]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i-(\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})(e^{\vec{w}\cdot\vec{x_i}+b})\frac{\partial}{\partial b}[\vec{w}\cdot\vec{x_i}+b]] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i-(\frac{1}{1+e^{\vec{w}\cdot\vec{x_i}+b}})(e^{\vec{w}\cdot\vec{x_i}+b})(1)] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i-(\frac{e^{\vec{w}\cdot\vec{x_i}+b}}{1+e^{\vec{w}\cdot\vec{x_i}+b}})] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i-(\frac{1}{1+e^{-}(\vec{w}\cdot\vec{x_i}+b)})] \\
&= -\frac{1}{n}\sum_{i=1}^{n}[y_i-\hat{y}_i] \\
&= \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i-y_i)
\end{aligned}$$

```
def bce_db(y_true, y_pred):
    return np.mean(y_pred - y_true)
```

0.4.8 Gradient Descent

With the binary cross entropy functions with respect to $\vec{w}$ and b, the gradient descent equations are:

Gradient Descent for weights $\vec{w}$

$$\begin{aligned}
\vec{w} &= \vec{w}-\eta\nabla_W[L(\vec{w},b)] \\
&= \vec{w}-\eta[\frac{1}{n}\sum_{i=1}^{n}[x_i(\hat{y}_i-y_i)]]
\end{aligned}$$

Gradient Descent for bias b

$$\begin{aligned} b &= b - \eta \frac{\partial}{\partial b}[L(\vec{w}, b)] \\ &= b - \eta[\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)] \end{aligned}$$

```
def gradient_descent(weights, x, bias, y_true, y_pred, learning_rate):
    weights = weights - learning_rate * bce_dw(x, y_true, y_pred)
    bias = bias - learning_rate * bce_db(y_true, y_pred)

    return weights, bias
```

0.4.9 Graphing functions

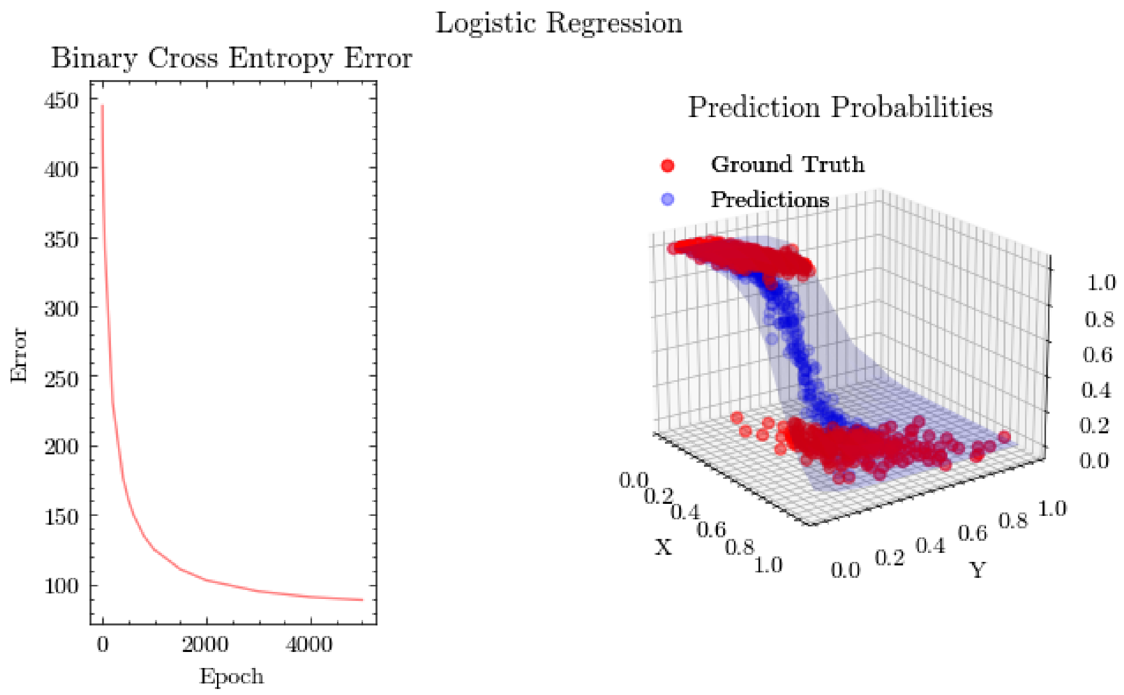
Utility functions to create the visualizations

```
def create_plots():
    fig, ax = plt.subplots(1, 3, figsize=(16 / 9.0 * 4, 4 * 1))
    fig.suptitle("Logistic Regression")

    ax[0].set_xlabel("Epoch", fontweight="normal")
    ax[0].set_ylabel("Error", fontweight="normal")
    ax[0].set_title("Binary Cross Entropy Error")

    ax[1].axis("off")
    ax[2].axis("off")

    ax[2] = fig.add_subplot(1, 2, 2, projection="3d")
    ax[2].set_xlabel("X")
    ax[2].set_ylabel("Y")
    ax[2].set_zlabel("Z")
    ax[2].set_title("Prediction Probabilities")
    ax[2].view_init(20, -35)

    camera = Camera(fig)
    return ax[0], ax[2], camera


def plot_graphs(
    ax0,
    ax1,
    idx,
    visible_mse,
    mse_idx,
    errors,
    features,
    labels,
    predictions,
    points_x,
    points_y,
    surface_predictions,
):
    ax0.plot(
        mse_idx[visible_mse][: idx + 1],
        errors[visible_mse][: idx + 1],
        color="red",
        alpha=0.5,
    )

    # Plot Logistic Regression Predictions
    # Ground truth and training data
    ground_truth_legend = ax1.scatter(
        features[:, 0],
        features[:, 1],
        labels,
        color="red",
        alpha=0.5,
        label="Ground Truth",
    )
    # Logistic Regression Predictions
    predictions_legend = ax1.scatter(
        features[:, 0],
        features[:, 1],
        predictions,
        color="blue",
        alpha=0.2,
        label="Prediction",
    )
    ax1.plot_surface(
        points_x,
        points_y,
        surface_predictions.reshape(dims, dims),
        color="blue",
        alpha=0.2,
    )
    ax1.legend(
        (ground_truth_legend, predictions_legend),
        ("Ground Truth", "Predictions"),
        loc="upper left",
    )
```

0.4.10 Training the model

```python
def fit(
    w0, b0, features, labels, dims, epochs, learning_rate, optimizer, output_filename
):
    mse_idx = np.arange(1, epochs + 1)
    errors = np.full(epochs, -1)
    ax0, ax1, camera = create_plots()

    points = np.linspace(0, 1, dims)
    points_x, points_y = np.meshgrid(points, points)
    surface_points = np.column_stack((points_x.flatten(), points_y.flatten()))

    weights = w0
    bias = b0

    for idx in range(epochs):
        error = 0
        predictions = np.array([])
        surface_predictions = np.array([])

        # fit the model on the training data
        for x, y in zip(features, labels):
            output = sigmoid(np.dot(weights, x) + bias)

            predictions = np.append(predictions, output)

            # Store Error
            error += bce(y, output)

            # Gradient Descent
            weights, bias = optimizer(weights, x, bias, y, output, learning_rate)

        # error /= len(features)

        # Visualization
        if (
            idx < 5
            or (idx < 15 and idx % 5 == 0)
            or (idx <= 50 and idx % 25 == 0)
            or (idx <= 1000 and idx % 200 == 0)
            or idx % 500 == 0
        ):
            for surface_point in surface_points:
                output = sigmoid(np.dot(weights, surface_point) + bias)
                surface_predictions = np.append(surface_predictions, output)

            print(f"epoch: {idx:>4}, BCA: {round(error, 2)}")

            # Plot BCE
            errors[idx] = error
            visible_mse = errors != -1

            plot_graphs(
                ax0,
                ax1,
                idx,
                visible_mse,
                mse_idx,
                errors,
                features,
                labels,
                predictions,
                points_x,
                points_y,
                surface_predictions,
            )

            camera.snap()

    animation = camera.animate()
    animation.save(output_filename, writer="pillow")
```

```python
epochs = 5001
learning_rate = 0.0005
dims = 10

w0 = np.random.rand(X[0].shape[0])
b0 = np.random.rand()

output_filename = "logistic_regression.gif"
fit(w0, b0, X, Y, dims, epochs, learning_rate, gradient_descent, output_filename)
```



0.5 Perceptron

The perceptron algorithm finds the optimal weights for a hyperplane to separate two classes, which is also known as binary classification.

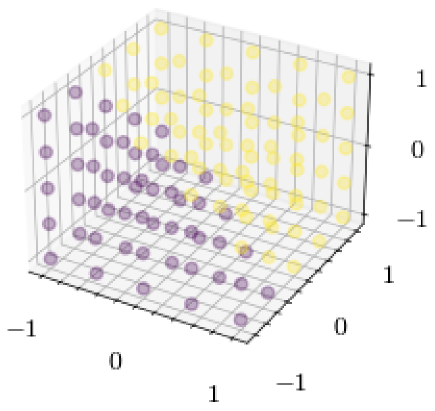
Import the libraries

```
import numpy as np

# %matplotlib ipympl
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

from celluloid import Camera
import scienceplots
from IPython.display import Image

np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

0.5.1 Training Dataset

Let's generate a dataset where the label is determined by a linear decision boundary. Our perceptron will layer find the weights of a normal vector to separate the dataset into two classes.

```
def generate_dataset(dims, normal_vector):
    # create 3D grid of points
    points = np.linspace(-1, 1, dims)
    X, Y, Z = np.meshgrid(points, points, points)

    # features are the x, y, z coordinates
    features = np.column_stack((X.ravel(), Y.ravel(), Z.ravel()))

    # labels are the side each point is on the hyperplane
    distances = np.dot(features, normal_vector)
    labels = np.where(distances >= 0, 1, -1)
    return X, Y, Z, features, labels

# normalized normal vector
target_normal_vector = np.array([1.0, 1.0, 1.0])
target_normal_vector = target_normal_vector / np.linalg.norm(target_normal_vector)

scaling = 5
X, Y, Z, features, labels = generate_dataset(scaling, target_normal_vector)

fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")

# plot the points
ax.scatter(features[:,0], features[:,1], features[:,2], marker='o', alpha=0.3, c=labels)
```



0.5.2 Hyperplane

A hyperplane is a flat subspace that is one less dimension than the current space. It can be used to linearly separate a dataset. The equation of a hyperplane is defined by the vector normal to the hyperplane $\vec{w}$

$$\vec{w} \cdot \vec{x} = w_1 x_1 + ... + w_n x_n = 0$$

In our case, the $\vec{x}$ is the x, y, z coordinate.

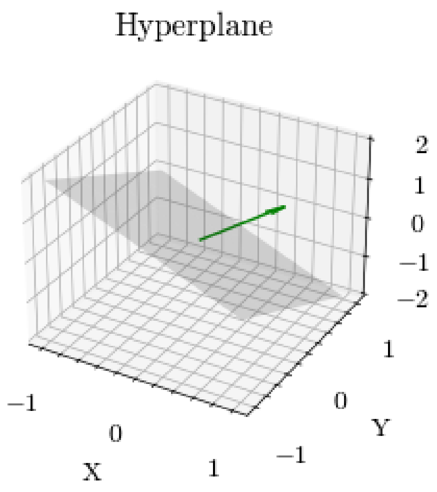
$$\begin{aligned} \vec{w} \cdot \vec{x} &= 0 \\ &= w_1 x + w_2 y + w_3 z \end{aligned}$$

Since we want to perform binary classification using the side a point is on relative from the hyperplane, the z value can be our predicted label

$$z = -(w_1 x + w_2 y)/w_3$$

```
def generate_hyperplane(scaling, normal_vector):
    # create 2D points
    points = np.linspace(-1, 1, scaling)
    xx, yy = np.meshgrid(points, points)

    # the z value is the defined by the hyperplane
    zz = -(normal_vector[0] * xx + normal_vector[1] * yy) / normal_vector[2]
    return xx, yy, zz

xx, yy, zz = generate_hyperplane(scaling, target_normal_vector)

# visualize the hyperplane
fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")

# plot the hyperplane defined by the normal vector
ax.plot_surface(xx, yy, zz, alpha=0.2, color="gray")
ax.quiver(
    0,
    0,
    0,
    target_normal_vector[0],
    target_normal_vector[1],
    target_normal_vector[2],
    color="green",
    length=1,
    arrow_length_ratio=0.2,
)

ax.set_xlabel("X")
ax.set_ylabel("Y")
ax.set_zlabel("Z")
ax.set_title("Hyperplane")
```

```
[3]: Text(0.5, 0.92, 'Hyperplane')
```



0.5.3 Loss Function: Hinge Loss

Loss functions are used to quantify the error of a prediction.

The perceptron uses the hinge loss function, which returns 0 for correct predictions and 1 for incorrect predictions.

$$L(\vec{w}, b) = max(0, -y(\vec{w} \cdot \vec{x} + b)$$

```
def hinge_loss(w, x, b, y):
    return max(0.0, -y * (np.dot(w, x) + b))
```

0.5.4 Hinge Loss Gradient

In order to run gradient descent to update our parameters, the gradients with respect to W and b must be calculated

0.5.5 Hinge Loss Gradient in Terms of B

Loss function with respect to b

$$\frac{\partial L}{\partial b} = \begin{cases} 0, & -y(\vec{w} \cdot \vec{x} + b) > 1 \\ -y, & \text{otherwise} \end{cases}$$

```
def hinge_loss_db(w, x, b, y):
    if y * (np.dot(w, x) + b) <= 0.0:
        return -y
    return 0
```

0.5.6 Hinge Loss Gradient in Terms of W

Loss function with respect to $\vec{w}$

$$\nabla\{W\}[L(\vec{w}, b)] = \begin{cases} 0, & -y(\vec{w} \cdot \vec{x} + b) > 1 \\ -y\vec{x}, & \text{otherwise} \end{cases}$$

```
def hinge_loss_dw(w, x, b, y):
    if y * (np.dot(w, x) + b) <= 0.0:
        return -y * x
    return np.zeros_like(x)
```

0.5.7 Graphing functions

Utility functions to create the visualizations

```python
def create_plots():
    fig, ax = plt.subplots(2, 3, figsize=(16 / 9.0 * 4, 4 * 1), layout="constrained")
    fig.suptitle("Perceptron")

    ax[0, 0].set_xlabel("Epoch", fontweight="normal")
    ax[0, 0].set_ylabel("Error", fontweight="normal")
    ax[0, 0].set_title("Hinge Loss")

    ax[1, 0].set_xlabel("Z, Distance to Hyperplane", fontweight="normal")
    ax[1, 0].set_ylabel("", fontweight="normal")
    ax[1, 0].set_title("Linear Transformation")

    ax[0, 1].axis("off")
    ax[0, 2].axis("off")
    ax[1, 1].axis("off")
    ax[1, 2].axis("off")

    ax[1, 2] = fig.add_subplot(1, 2, 2, projection="3d")
    ax[1, 2].set_xlabel("X")
    ax[1, 2].set_ylabel("Y")
    ax[1, 2].set_zlabel("Z")
    ax[1, 2].set_title("Hyperplane Decision Boundary")
    ax[1, 2].view_init(20, -35)
    ax[1, 2].set_xlim(-1, 1)
    ax[1, 2].set_ylim(-1, 1)
    ax[1, 2].set_zlim(-1, 1)

    camera = Camera(fig)
    return ax[0, 0], ax[1, 0], ax[1, 2], camera


def plot_graphs(
    ax0,
    ax1,
    ax2,
    idx,
    visible_err,
    err_idx,
    errors,
    scaling,
    target_normal_vector,
    predictions,
    features,
    labels,
    weights,
):
    ax0.plot(
        err_idx[visible_err][: idx + 1],
        errors[visible_err][: idx + 1],
        color="red",
    )

    # Ground truth
    xx_target, yy_target, zz_target = generate_hyperplane(scaling, target_normal_vector)
    ground_truth_legend = ax2.plot_surface(
        xx_target,
        yy_target,
        zz_target,
        color="red",
        alpha=0.2,
        label="Ground Truth",
    )
    ax2.quiver(
        0,
        0,
        0,
        target_normal_vector[0],
        target_normal_vector[1],
        target_normal_vector[2],
        color="red",
        length=1,
        arrow_length_ratio=0.1,
    )

    # Perceptron predictions using 2D graph to show linear transformation
    def generate_colors(arr):
        return ["green" if d >= 0 else "orange" for d in arr]

    ground_truth_colors = generate_colors(labels)
    ax1.scatter(
        predictions,
        np.zeros(predictions.shape),
        c=ground_truth_colors,
        marker="o",
        alpha=0.3,
    )

    # Perceptron predictions using 3D graph to show hyperplane
    predictions_colors = generate_colors(predictions)
    predictions_norm = np.maximum(1 - np.exp(-(predictions**2)), 0.2)

    ax2.scatter(
        features[:, 0],
        features[:, 1],
        features[:, 2],
        c=predictions_colors,
        marker="o",
        alpha=predictions_norm,
    )

    xx, yy, zz = generate_hyperplane(scaling, weights)
    predictions_legend = ax2.plot_surface(
        xx,
        yy,
        zz,
        color="blue",
        alpha=0.2,
        label="Prediction",
    )
    ax2.quiver(
        0,
        0,
        0,
        weights[0],
        weights[1],
        weights[2],
        color="blue",
        length=1,
        arrow_length_ratio=0.1,
```

0.5.8 Gradient Descent

Gradient Descent will be used to update the weights and bias.

Bias Gradient Descent:

$$\begin{aligned} b &= b - \eta \frac{\partial}{\partial b}[L(\vec{w}, b)] \\ &= b - \eta \begin{cases} 0 & -y(\vec{w} \cdot \vec{x} + b) > 1 \\ -y & \text{otherwise} \end{cases} \end{aligned}$$

Weights Gradient Descent:

$$\begin{aligned} \vec{w} &= \vec{w} - \eta \nabla_W [L(\vec{w}, b)] \\ &= \vec{w} - \eta \begin{cases} 0 & -y(\vec{w} \cdot \vec{x} + b) > 1 \\ -yx & \text{otherwise} \end{cases} \end{aligned}$$

```
def gradient_descent(weights, x, bias, y, learning_rate):
    weights = weights - learning_rate * hinge_loss_dw(weights, x, bias, y)
    bias = bias - learning_rate * hinge_loss_db(weights, x, bias, y)

    return weights, bias
```

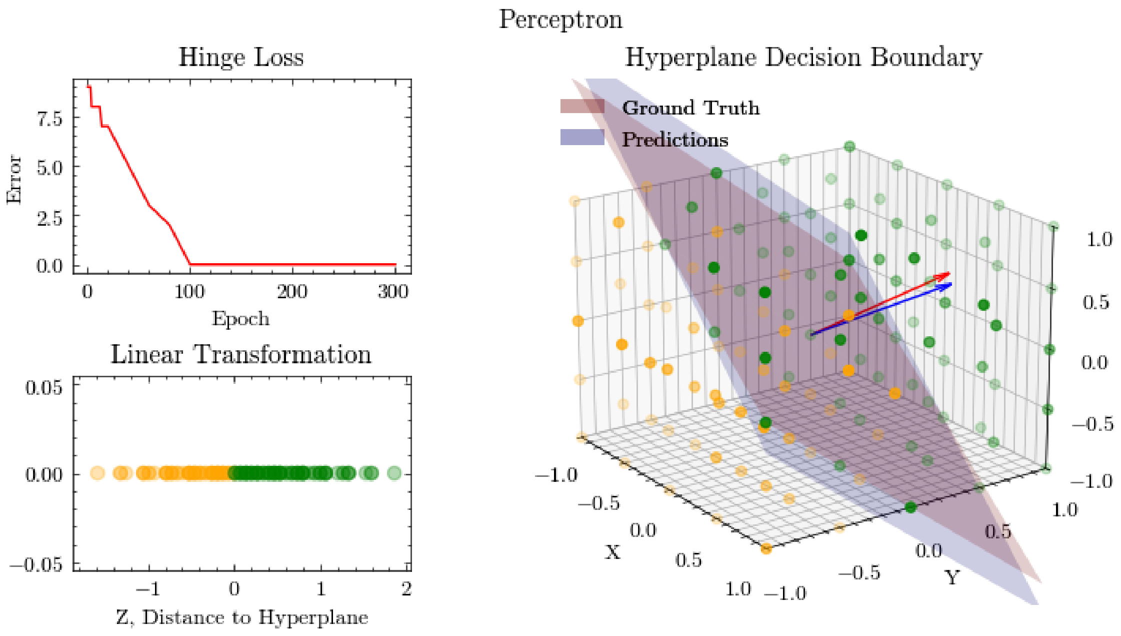
0.5.9 Training the Model

```
def fit(
    weights,
    bias,
    target_normal_vector,
    features,
    labels,
    X,
    Y,
    Z,
    scaling,
    epochs,
    learning_rate,
    optimizer,
    output_filename,
):
    err_idx = np.arange(1, epochs + 1)
    errors = np.full(epochs, -1)
    ax0, ax1, ax2, camera = create_plots()

    for idx in range(epochs):
        error = 0
        predictions = np.array([])

        for x, y in zip(features, labels):
            # Forward Propagation
            output = np.dot(weights, x) + bias

            predictions = np.append(predictions, output)

            # Store Error
            error += hinge_loss(weights, x, bias, y)

            # Gradient Descent
            weights, bias = optimizer(weights, x, bias, y, learning_rate)

        error /= len(X)
        weights = weights / np.linalg.norm(weights)

        if (
            idx < 5
            or (idx < 15 and idx % 2 == 0)
            or (idx <= 50 and idx % 10 == 0)
            or (idx <= 1000 and idx % 20 == 0)
            or idx % 250 == 0
        ):

            print(f"epoch: {idx}, MSE: {error}")

            # Plot MSE
            errors[idx] = error
            visible_err = errors != -1

            plot_graphs(
                ax0,
                ax1,
                ax2,
                idx,
                visible_err,
                err_idx,
                errors,
                scaling,
                target_normal_vector,
                predictions,
                features,
                labels,
                weights,
            )

            camera.snap()

    animation = camera.animate()
    animation.save(output_filename, writer="pillow")
    plt.show()
```

Let's put everything together and train our Perceptron

```
weights = np.array([1.0, -1.0, -1.0])
weights = weights / np.linalg.norm(weights)

bias = 0
```

```
epochs = 301
learning_rate = 0.0005

output_filename = "perceptron.gif"
fit(
    weights,
    bias,
    target_normal_vector,
    features,
    labels,
    X,
    Y,
    Z,
    scaling,
    epochs,
    learning_rate,
    gradient_descent,
    output_filename,
)
```



0.6 Neural Network Weights Visualization

Neural Networks at a high-level just consist of matrix multiplications at each layer. Matrix multiplications are linear transformations. This visualization shows the linear transformations at each layer and the loss landscape of each layer. This Notebook builds on top of the `Neural Network` Notebook. Look at the previous Notebook for the derivation of Backpropagation and the math behind neural networks.

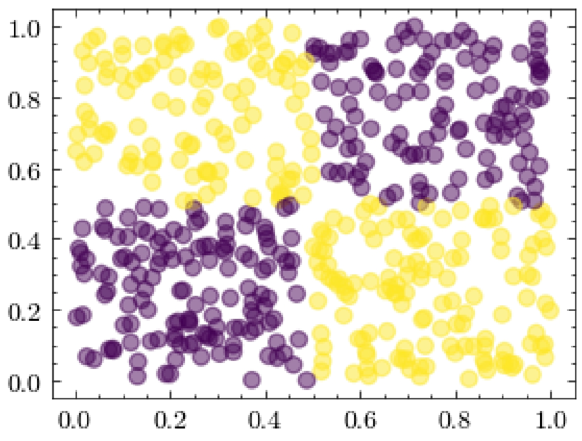
Gavin's Note: The goal of this visualization is show that Backpropagation updates the weights and biases in the most optimal way. In order to visualize this, this program changes the weights to make them non optimal to show that the loss increases. As a result, this program will take a very long time.

```
import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F

# %matplotlib ipympl
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

from celluloid import Camera
import scienceplots
from IPython.display import Image

torch.manual_seed(0)
np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

0.6.1 Training Dataset

Let's generate a non-linear dataset, since neural networks can fit this function while linear models, such as a perceptron, can't converge on this dataset

```
# generate the non-linear dataset, meaning that a hyperplane can't separate the data
def generate_XOR():
    N = 500
    X = np.random.rand(N, 2)
    y = (X[:, 0] > 0.5) != (X[:, 1] > 0.5)

    return X, y


X, y = generate_XOR()

fig = plt.figure()
ax = fig.add_subplot()
ax.scatter(X[:, 0], X[:, 1], c=y, alpha=0.5)
```



0.6.2 Graph Functions

In our training function, we use the gradient descent optimizer to update the weights and move on. What if we didn't use the weights from the optimizer? These graphing functions manually change the values in the weight matrix of our neural network's layers and run the neural network to see how the loss changes.

There are also graphing functions that show the linear transformation of each layer.

```python
def create_scatterplots(rows=2, cols=3, width_scale=1, height_scale=1):
    fig, axes = plt.subplots(
        rows,
        cols,
        figsize=(16 / 9.0 * 4 * width_scale, 4 * height_scale),
        layout="constrained",
    )
    axes = axes.flatten()

    layer_idx = 0
    for i, axis in enumerate(axes):
        if not ((i + 1) % cols == 0):
            axis.set_title(f"Layer {layer_idx}")
            layer_idx += 1

    axes[-1].set_title("Predictions")
    axes[-1 - cols].set_title("Mean Squared Error")

    camera = Camera(fig)
    return axes, camera


def create_3d_plots(rows=2, cols=3, width_scale=1, height_scale=1):
    fig = plt.figure(
        figsize=(16 / 9.0 * 4 * width_scale, 4 * height_scale), layout="constrained"
    )
    axes = []

    layer_idx = 0
    for i in range(rows * cols):
        if not ((i + 1) % cols == 0):
            axis = fig.add_subplot(rows, cols, i + 1, projection="3d")
            axis.set_title(f"Layer {layer_idx + 1}")
            axes.append(axis)
            layer_idx += 1
        else:
            axes.append(fig.add_subplot(rows, cols, i + 1))

    axes[-1].set_title("Predictions")
    axes[-1 - cols].set_title("Mean Squared Error")

    camera = Camera(fig)
    return axes, camera


def plot_layer_loss_landscape(
    axis,
    model,
    target_layer_idx,
    neuron_idx,
    features,
    labels,
    w1_min,
    w1_max,
    w2_min,
    w2_max,
    loss_dims,
    device,
    color="blue",
):
    """Plot how the loss changes when the first two weights in the first neuron change"""
    loss_fn = nn.MSELoss()

    init = model.get_values(target_layer_idx, neuron_idx)
    w1 = init[0].item()
    w2 = init[1].item()

    target_layer_idx = target_layer_idx % len(model.layers)

    w1_range = torch.linspace(w1_min + w1, w1_max + w1, loss_dims).to(device)
    w2_range = torch.linspace(w2_min + w2, w2_max + w2, loss_dims).to(device)
    w1_range, w2_range = torch.meshgrid(w1_range, w2_range, indexing="ij")
    w_range = torch.stack((w1_range.flatten(), w2_range.flatten()), axis=1)

    error_range = np.array([])

    for target_layer_weight in w_range:
        model.override_layer_weight(
            target_layer_idx, neuron_idx, init + target_layer_weight
        )
        error = 0
        for x, y in zip(features, labels):
            output = model(x)
            y = y.unsqueeze(0)
            loss = loss_fn(output, y)
            error += loss.detach().cpu().numpy()
        error /= len(labels)
        error_range = np.append(error_range, error)

        if np.isclose(target_layer_weight[0].item(), w1, atol=0.25) and np.isclose(
            target_layer_weight[1].item(), w2, atol=0.25
        ):
            axis.scatter([w1], [w2], [error], color=color, alpha=0.4)

    axis.plot_surface(
        w1_range.detach().cpu().numpy(),
        w2_range.detach().cpu().numpy(),
        error_range.reshape(loss_dims, loss_dims),
        color=color,
        alpha=0.1,
    )
    model.override_layer_weight(target_layer_idx, neuron_idx, init)


def plot_mse_and_predictions(
    axes, features, idx, visible_mse, mse_idx, errors, predictions, cmap, cols, device
):
    features_cpu = features.detach().cpu().numpy()

    # Plot MSE
    mse_ax = axes[-1 - cols]
    mse_ax.plot(
        mse_idx[visible_mse][: idx + 1],
        errors[visible_mse][: idx + 1],
        color="red",
        alpha=0.5,
    )
    mse_ax.plot(
        [1],
```

0.6.3 PyTorch Implementation

Let's define a feedforward neural network in PyTorch, but add custom functions to each layer that manually change the weight values. We want to use this function to see how the loss changes when the weights aren't at the optimal value. This is used to show that Backpropagation tells us how to update the weights optimally.

```
class VisualNet(nn.Module):
    def __init__(self):
        super(VisualNet, self).__init__()
        self.layers = nn.ModuleList()

    def visualize(self, X, y, axes, cmap, rows, cols):
        y_cpu = y.detach().cpu().numpy()

        layer_idx = 0
        for i, axis in enumerate(axes):
            if not ((i + 1) % cols == 0):
                X_cpu = X.detach().cpu().numpy()

                # input and hidden layer outputs
                if X.shape[1] != 1:
                    axis.scatter(
                        X_cpu[:, 0], X_cpu[:, 1], c=y_cpu, cmap=cmap, alpha=0.5
                    )
                # output layer is 1D, so set second dimenstional to zeros
                else:
                    axis.scatter(
                        X_cpu[:, 0],
                        np.zeros(X_cpu[:, 0].shape),
                        c=y_cpu,
                        cmap=cmap,
                        alpha=0.5,
                    )

                if layer_idx < len(self.layers):
                    X = F.tanh(self.layers[layer_idx](X))
                    layer_idx += 1

    def override_layer_weight(self, layer_idx, neuron_idx, new_weights):
        if (abs(layer_idx) > len(self.layers)) or (
            abs(neuron_idx) > len(self.layers[layer_idx].weight)
        ):
            return

        with torch.no_grad():
            self.layers[layer_idx].weight[neuron_idx, :2] = new_weights

    def get_values(self, layer_idx, neuron_idx):
        if (abs(layer_idx) > len(self.layers)) or (
            abs(neuron_idx) > len(self.layers[layer_idx].weight)
        ):
            return torch.zeros(2)

        with torch.no_grad():
            return self.layers[layer_idx].weight.detach().clone()[neuron_idx, :2]


class TorchNet(VisualNet):
    def __init__(self, num_hidden_layers):
        super().__init__()

        # define the layers
        self.input_layer = nn.Linear(2, 2)
        self.layers.append(self.input_layer)

        for i in range(num_hidden_layers):
            self.layers.append(nn.Linear(2, 2))

        self.output_layer = nn.Linear(2, 1)
        self.layers.append(self.output_layer)

    def forward(self, x):
        # pass the result of the previous layer to the next layer
        for layer in self.layers[:-1]:
            x = F.tanh(layer(x))

        return self.output_layer(x)
```

0.6.4 Training the Model

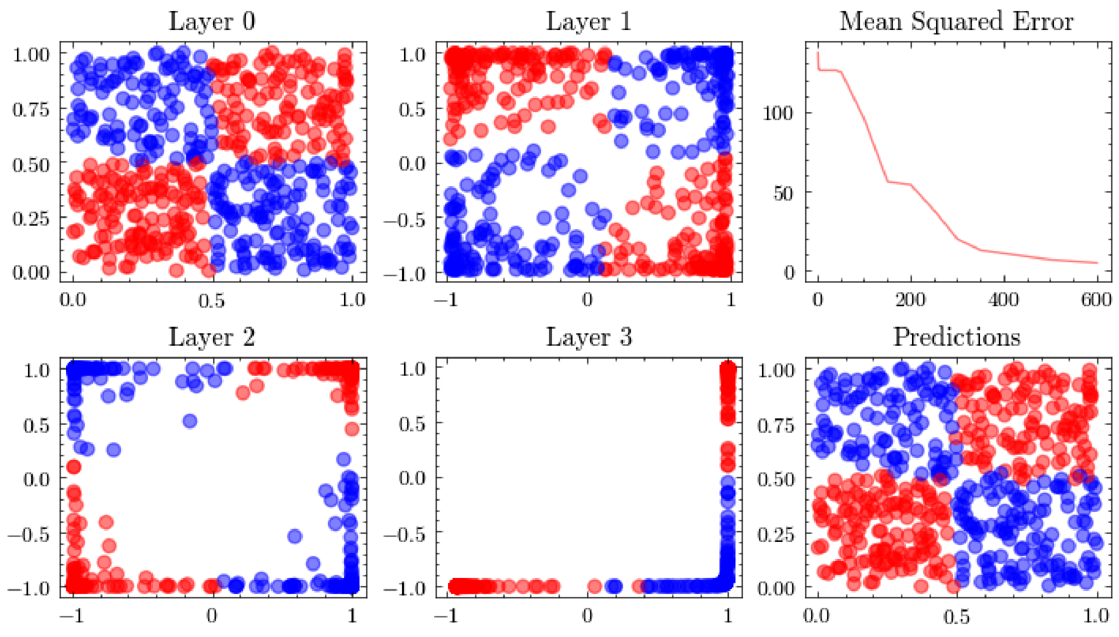
Similar to the previous Neural Network Notebook, let's pass in the training data to our model, update the weights with our optimizer, and update our visualization

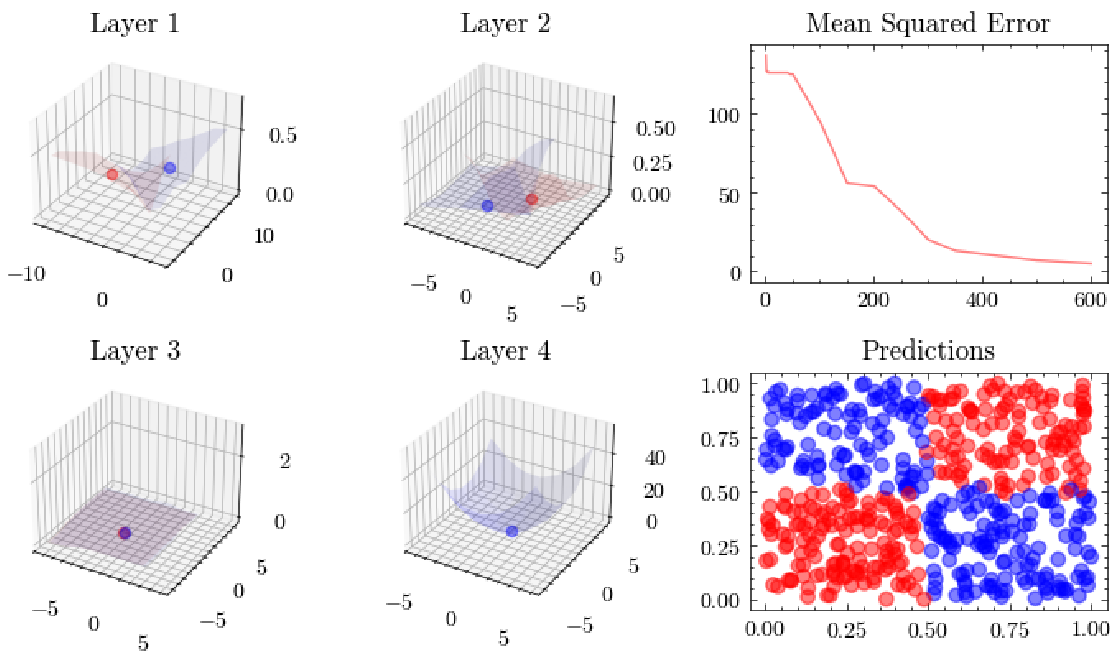
```python
def torch_fit(
    model,
    features,
    labels,
    epochs,
    learning_rate,
    transformations_plot_filename,
    loss_landscape_plot_filename,
    device,
    rows=2,
    cols=3,
    width_scale=1,
    height_scale=1,
):
    mse_idx = np.arange(1, epochs + 1)
    errors = np.full(epochs, -1)

    cmap = plt.cm.colors.ListedColormap(["red", "blue"])

    scatterplots, camera1 = create_scatterplots(rows, cols, width_scale, height_scale)
    loss_plots, camera2 = create_3d_plots(rows, cols, width_scale, height_scale)

    loss_fn = nn.MSELoss()
    optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate, momentum=0.3)

    for idx in range(epochs):
        error = 0
        predictions = np.array([])

        for x, y in zip(features, labels):
            # Forward Propagation
            output = model(x)

            output_np = output.detach().cpu().numpy()
            predictions = np.append(predictions, output_np)

            # Store Error
            # tensor(0.) -> tensor([0.]) to match shape of output variable
            y = y.unsqueeze(0)
            loss = loss_fn(output, y)

            error += loss.detach().cpu().numpy()

            # Backpropagation
            optimizer.zero_grad()
            loss.backward()
            optimizer.step()

        if (
            idx < 5
            or (idx <= 50 and idx % 5 == 0)
            or (idx <= 1000 and idx % 50 == 0)
            or idx % 250 == 0
        ):
            print(f"epoch: {idx}, MSE: {error}")

            # Plot MSE
            errors[idx] = error
            visible_mse = errors != -1

            plot_transformations_and_predictions(
                scatterplots,
                model,
                idx,
                visible_mse,
                mse_idx,
                errors,
                predictions,
                features,
                labels,
                cmap,
                rows,
                cols,
                device,
            )

            plot_loss_landscape_and_predictions(
                loss_plots,
                model,
                idx,
                visible_mse,
                mse_idx,
                errors,
                predictions,
                features,
                labels,
                cmap,
                cols,
                device,
            )

            camera1.snap()
            camera2.snap()

    animation1 = camera1.animate()
    animation1.save(transformations_plot_filename, writer="pillow")
    animation2 = camera2.animate()
    animation2.save(loss_landscape_plot_filename, writer="pillow")

    plt.show()
```

0.6.5 Visualize the transformations and weight updates

Let's call our training function with our model to create the visualization.

```
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
torch_model = TorchNet(num_hidden_layers=2).to(device)

rows = 2
cols = 3

# the inputs and outputs for PyTorch must be tensors
X_tensor = torch.tensor(X, device=device, dtype=torch.float32).squeeze(-1)
y_tensor = torch.tensor(y, device=device, dtype=torch.float32).squeeze(-1)

epochs = 601
learning_rate = 0.005

transformations_plot_filename = "neural_network_weights.gif"
loss_landscape_plot_filename = "neural_network_weights_loss_landscape.gif"
torch_fit(
    torch_model,
    X_tensor,
    y_tensor,
    epochs,
    learning_rate,
    transformations_plot_filename,
    loss_landscape_plot_filename,
    device,
    rows=rows,
    cols=cols,
)
```





This visualization shows the internal linear transformation of each layer in the neural network. We will show each layer transform an input to an output. At the 3rd layer, the data becomes linearly separable. As a result of these transformations, the network is able to classify inputs into these two classes.

This visualization shows that the weights all update together such that the loss function at the last layer reaches the minima. See how the 3D plot in layer 4 is at a minima.

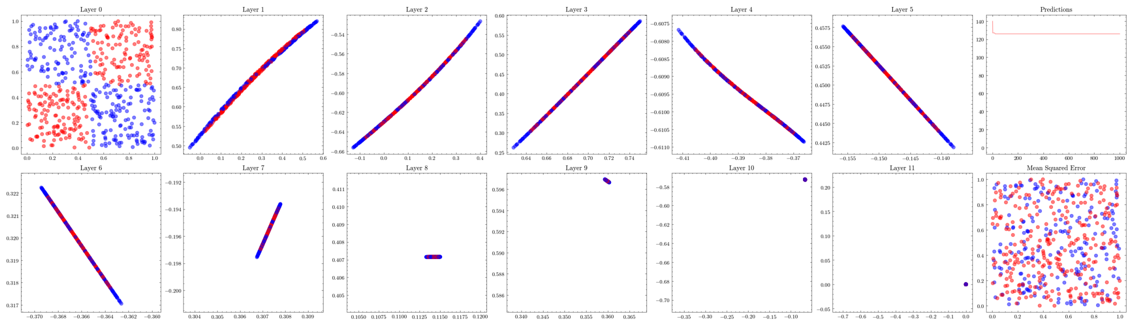
0.6.6 Vanishing Gradients

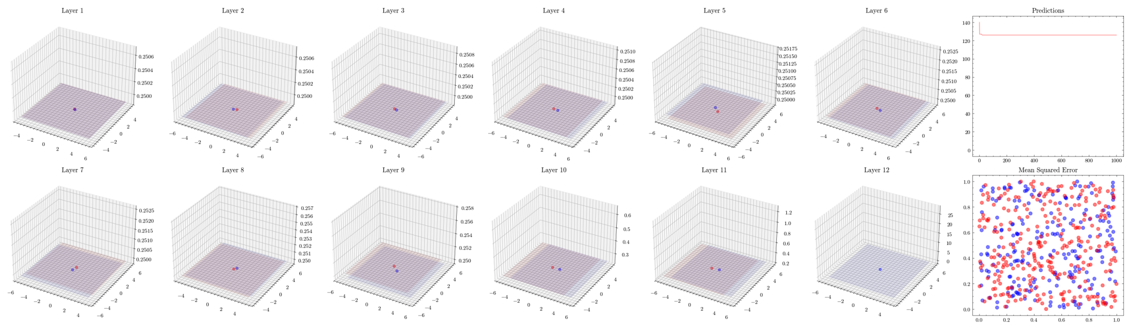
It's a valid assumption that increasing the number of layers of a neural network allows it to recognize more patterns. However, scaling is not this straightforward. With the wrong architectures, the networks can stop scaling. The next visualization increases the number of layers to 12 and shows that the weights can not update. This is known as vanishing gradients since the updates being sent to the earlier layers in the network are close to zero, preventing the weights from updating. The ResNet paper introduced residual connections, which helped solved this issue.

12 Layer Neural Network

Let's rerun our code but with a larger network this time

```
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
torch_model = TorchNet(num_hidden_layers=10).to(device)

rows = 2
cols = 7

X_tensor = torch.tensor(X, device=device, dtype=torch.float32).squeeze(-1)
y_tensor = torch.tensor(y, device=device, dtype=torch.float32).squeeze(-1)

epochs = 1001
learning_rate = 0.005

width_scale = 4
height_scale = 2

transformations_plot_filename = "vanishing_gradients/layers_12.gif"
loss_landscape_plot_filename = "vanishing_gradients/layers_12_loss_landscape.gif"
torch_fit(
    torch_model,
    X_tensor,
    y_tensor,
    epochs,
    learning_rate,
    transformations_plot_filename,
    loss_landscape_plot_filename,
    device,
    rows=rows,
    cols=cols,
    width_scale=width_scale,
    height_scale=height_scale,
)
```





In the visualizations below, we see the earlier layers not updating at all from vanishing gradients.

0.7 Neural Network

Neural Networks are a machine learning model that learns the optimal parameters to approximate complex functions.

GitHub Repo: https://github.com/gavinkhung/neural-network

Import the libraries

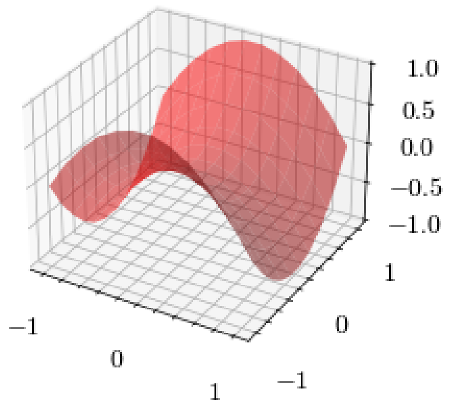
```
import numpy as np

%matplotlib ipympl
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

from celluloid import Camera
import scienceplots
from IPython.display import Image

np.random.seed(0)
plt.style.use(["science", "no-latex"])
```

0.7.1 Training Dataset

The neural network will learn the parameters to fit a Hyperbolic Paraboloid.

$$z = \frac{y^2}{b^2} - \frac{x^2}{a^2}$$

```
def generate_function(dims):
    a = 1
    b = 1

    # Hyperbolic Paraboloid
    x = np.linspace(-1, 1, dims)
    y = np.linspace(-1, 1, dims)
    X, Y = np.meshgrid(x, y)
    Z = (Y**2 / b**2) - (X**2 / a**2)

    X_t = X.flatten()
    Y_t = Y.flatten()
    Z_t = Z.flatten()
    X_t = X_t.reshape((len(X_t), 1))
    Y_t = Y_t.reshape((len(Y_t), 1))
    Z_t = Z_t.reshape((len(Z_t), 1))
    features = np.stack((X_t, Y_t), axis=1)
    labels = Z_t.reshape((len(Z_t), 1, 1))

    return X, Y, Z, features, labels


dims = 12
X, Y, Z, features, labels = generate_function(dims)

# Visualize the Hyperbolic Paraboloid
fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")

ax.plot_surface(X, Y, Z, color="red", alpha=0.5)
```



0.7.2 Loss Function

The loss function is needed to evaluate the performance of the model and to update the weights accordingly. The optimizaton process of the neural network training will find the weights and biases to minimie the loss.

Mean Squared Error

Quadratic loss functions, like mean squared error, are used for regression tasks, like this example.

$$J = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

```
def mse(y_true, y_pred):
    return np.mean(np.power(y_true - y_pred, 2))
```

Mean Squared Error Gradient

In order to perform backpropagation to update the weights, we need to calculate the gradient of the loss function.

$$\begin{aligned}
J' &= \frac{\partial}{\partial \hat{y}}[\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y})^2] \\
&= \frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial \hat{y}}[(y_i - \hat{y})^2] \\
&= \frac{2}{n}\sum_{i=1}^{n}(y_i - \hat{y})\frac{\partial}{\partial \hat{y}}[y_i - \hat{y}] \\
&= \frac{2}{n}\sum_{i=1}^{n}(y_i - \hat{y})(-1) \\
&= \frac{2}{n}\sum_{i=1}^{n}(\hat{y} - y_i)
\end{aligned}$$

```
def mse_prime(y_true, y_pred):
    return 2 * (y_pred - y_true) / np.size(y_true)
```

0.7.3 Neural Network Layer

We will implement a feedforward neural network, which contains many layers. Each layer at a very high applies a linear transformation to the input data to create the output data, which is often in a different dimension than the input data. Then, all of the values in the output are run through a function, known as an activation function.

Recall from Linear Algebra that an input column vector x in $\mathbb{R}^n$ can be transformed into another dimension $\mathbb{R}^m$ by multipying it with a matrix of size $m \times n$. Finally we can add a bias term to this linear transformation to shift the transformed data up or down.

As a result, each layer stores a weight matrix and a bias vector to apply the linear transformation.

```python
from abc import ABC, abstractmethod


class Layer(ABC):
    def __init__(self):
        self.input = None
        self.output = None
        self.weights = None
        self.bias = None

    @abstractmethod
    def forward(self, input):
        pass

    @abstractmethod
    def backward(self, output_gradient, optimizer):
        pass
```

0.7.4 Forward Propagation

This the process of transforming our input data into the predictions from our feedforward neural network. The input data is passed through every layer of the network.

Each neuron in a layer is a weighted sum of its inputs plus a bias term. Finally, an activation function is applied on each neuron in the layer. We will have a class to represent a fully-connected layer and another class to represent an activation function.

The computation for each neuron in a layer being a weighted sum of the products between the inputs and the layer's weights plus a bias term is the same as a matrix multiplication between the weight matrix and the input data added with a bias vector.

Thus, the forward propagation of a fully connected layer can be written as:

$$\begin{aligned} Z &= WX + B \\ A &= g(Z) \end{aligned}$$

Where: - W is the weight matrix for the layer - X is the input data - B is a bias vector - g is the activation function

0.7.5 Our Network's Forward Propagation

We will implement a 3-layer fully-connected neural network with a Tanh activation function after each layer. These transformations can be written as these matrix multiplications:

$$\begin{aligned} Z_1 &= W_1X + B_1 \\ A_1 &= tanh(Z_1) \\ \\ Z_2 &= W_2A_1 + B_2 \\ A_2 &= tanh(Z_2) \\ \\ Z_3 &= W_3A_2 + B_3 \\ \hat{y} &= A_3 = tanh(Z_3) \end{aligned}$$

0.7.6 Backpropagation

Backpropagation is the process of updating all of the weights and biases in a neural network using the chain rule and gradient descent.

The following equations use J as our loss function. In this Notebook, we use the mean squared error loss function. Click here for the mean squared error loss function.

Our goal is to apply gradient descent on the weights and bias using the following equations:

$$\begin{aligned}
W_1 &= W_1 - lr * \frac{\partial J}{\partial W_1} \\
B_1 &= B_1 - lr * \frac{\partial J}{\partial B_1} \\
W_2 &= W_2 - lr * \frac{\partial J}{\partial W_2} \\
B_2 &= B_2 - lr * \frac{\partial J}{\partial B_2} \\
W_3 &= W_3 - lr * \frac{\partial J}{\partial W_3} \\
B_3 &= B_3 - lr * \frac{\partial J}{\partial B_3}
\end{aligned}$$

We need to use the chain rule to get the values for $\frac{\partial J}{\partial W_1}$, $\frac{\partial J}{\partial B_1}$, $\frac{\partial J}{\partial W_2}$, $\frac{\partial J}{\partial B_2}$, $\frac{\partial J}{\partial W_3}$, and $\frac{\partial J}{\partial B_3}$.

Chain Rule for Backpropagation

Let's derive a general formula to update the weight matrix W_i and bias vector B_i of a single fully-connected layer.

To apply gradient descent on the 3rd layer, for example, we need to find the loss with respect to W_3 and B_3, which are $\frac{\partial J}{\partial W_3}$, and $\frac{\partial J}{\partial B_3}$.

The loss function J is in terms of A_3, which is the final output/activation of the last layer. Then, A_3 is in terms of Z_3. Lastly, Z_3 is in terms of W_3, B_3, and A_2, which is the activation from the second to last layer. Let's get the loss with respect to W_3 and B_3.

We can represent these matrix operations as the following composite functions: $J(A_3)$, $A_3(Z_3)$, and $Z_3(W_3, B_3, A_2)$

Click here for the operations of each layer.

Chain Rule For Weight Matrix W

Use the chain rule to derive $\frac{\partial J}{\partial W_3}$

$$\begin{aligned}
\frac{\partial J}{\partial W_3} &= \frac{\partial}{\partial W_3}[J(A_3(Z_3(W_3, B_3, A_2)))] \\
&= \frac{\partial J}{\partial A_3}\frac{\partial}{\partial W_3}[A_3(Z_3(W_3, B_3, A_2))] \\
&= \frac{\partial J}{\partial A_3}\frac{\partial A_3}{\partial Z_3}\frac{\partial}{\partial W_3}[Z_3(W_3, B_3, A_2))] \\
&= \frac{\partial J}{\partial A_3}\frac{\partial A_3}{\partial Z_3}\frac{\partial Z_3}{\partial W_3}
\end{aligned}$$

Chain Rule For Bias Vector B

Use the chain rule to derive $\frac{\partial J}{\partial B_3}$.

$$\begin{aligned}
\frac{\partial J}{\partial B_3} &= \frac{\partial}{\partial B_3}[J(A_3(Z_3(W_3, B_3, A_2)))] \\
&= \frac{\partial J}{\partial A_3}\frac{\partial}{\partial B_3}[A_3(Z_3(W_3, B_3, A_2))] \\
&= \frac{\partial J}{\partial A_3}\frac{\partial A_3}{\partial B_3}\frac{\partial}{\partial B_3}[Z_3(W_3, B_3, A_2))] \\
&= \frac{\partial J}{\partial A_3}\frac{\partial A_3}{\partial Z_3}\frac{\partial Z_3}{\partial B_3}
\end{aligned}$$

0.7.7 Backpropagation for Weight Matrix W

$$\frac{\partial J}{\partial W_3} = \frac{\partial J}{\partial A_3}\frac{\partial A_3}{\partial Z_3}\frac{\partial Z_3}{\partial W_3}$$

Let's break each component down:

1. $\frac{\partial J}{\partial A_3}$ is the gradient of the loss function, which is the gradient of the mean squared error function. Click here for the derivation of the loss function gradient. In the general case for any layer, this is the gradient from the next layer (idx+1).

2. $$\frac{\partial A_3}{\partial Z_3} = \frac{\partial}{\partial Z_3}[tanh(Z\_3)]$$
   is the gradient of the activation function. Click here for the derivation of the activation function gradient.

3. $\frac{\partial Z_3}{\partial W_3} = \frac{\partial}{\partial W_3}[W_3 A_2 + B_3] = A_2$ is the original input to the layer, which is the output of the previous layer (idx-1).

As a result, to the gradient of the weight matrix of a fully-connected layer is the matrix multiplication products of the following: 1. The gradient from the next layer (idx+1) 2. The gradient of the activation function 3. The input from the previous layer (idx-1)

0.7.8 Backpropagation for Bias Vector B

$$\frac{\partial J}{\partial B_3} = \frac{\partial J}{\partial A_3}\frac{\partial A_3}{\partial Z_3}\frac{\partial Z_3}{\partial B_3}$$

Let's break each component down:

1. $\frac{\partial J}{\partial A_3}$ is the gradient of the loss function, which is the gradient of the mean squared error function. Click here for the derivation of the loss function gradient. In the general case for any layer, this is the gradient from the next layer (idx+1).

2. $\frac{\partial A_3}{\partial Z_3}$ is the gradient of the activation function. Click here for the derivation of the activation function gradient.

3. $\frac{\partial Z_3}{\partial B_3} = \frac{\partial}{\partial B_3}[W_3 A_2 + B_3] = 1$ is 1, we can ignore this in the gradient computation.

As a result, to the gradient of the bias vector of a fully-connected layer is the matrix multiplication products of the following: 1. The gradient from the next layer (idx+1) 2. The gradient of the activation function

For more information, I recommend the follow resources: - Neural Network from Scratch. I also watched this video to help write this Notebook. - The Most Important Algorithm in Machine Learning

0.7.9 Dense Layers

A dense layer is a fully connected layer. Let's use the equations derived in the forward and backwards propagation sections above to implement the `forward()` and `backward()` methods of our dense layer class.

```
class Dense(Layer):
    def __init__(self, input_neurons, output_neurons):
        # Random Values from Normal Distribution
        # self.weights = np.random.randn(output_neurons, input_neurons)
        # self.bias = np.random.randn(output_neurons, 1)

        # All Zeros
        # self.weights = np.zeros((output_neurons, input_neurons))
        # self.bias = np.zeros((output_neurons, 1))

        # Xavier Initialization Uniform Distribution
        limit = np.sqrt(6 / (input_neurons + output_neurons))
        self.weights = np.random.uniform(
            -limit, limit, size=(output_neurons, input_neurons)
        )
        self.bias = np.zeros((output_neurons, 1))

    def forward(self, input):
        self.input = input
        return np.matmul(self.weights, self.input) + self.bias

    def backward(self, output_gradient, optimizer):
        # Calculate gradients
        weights_gradient = np.matmul(output_gradient, self.input.T)
        input_gradient = np.dot(self.weights.T, output_gradient)

        # Update weights and biases
        self.weights, self.bias = optimizer.backward(
            self.weights, weights_gradient, self.bias, output_gradient
        )
        return input_gradient
```

0.7.10 Activation Function

Activation functions are applied after the matrix multiplication to introduce nonlinearity into our neural networks. Choosing the correct activation function is essential for the neural network to learn general patterns of the training data. Most notably, the ReLU function is very useful when training very deep neural networks with many layers, as seen from the 2012 AlexNet paper, in order to prevent vanishing gradients, where the network fails to update its weights from super small gradients

```
class Activation(Layer):
    def __init__(self, activation, activation_prime):
        self.activation = activation
        self.activation_prime = activation_prime

    def forward(self, input_val):
        self.input = input_val
        return self.activation(self.input)

    def backward(self, output_gradient, optimizer):
        return np.multiply(output_gradient, self.activation_prime(self.input))

    def plot(self, x_min, x_max, points=25):
        x = np.linspace(x_min, x_max, points)
        y = self.activation(x)
        y_prime = self.activation_prime(y)

        fig, axes = plt.subplots(1, 2)
        axes[0].plot(x, y)
        axes[0].set_xlabel("X")
        axes[0].set_ylabel("Y")
        axes[0].set_title("F(X)")

        axes[1].plot(x, y_prime)
        axes[1].set_xlabel("X")
        axes[1].set_ylabel("Y")
        axes[1].set_title("F'(X)")
```

Tanh Activation Function

We will use the Tanh activation function for our network:

$$\sigma(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

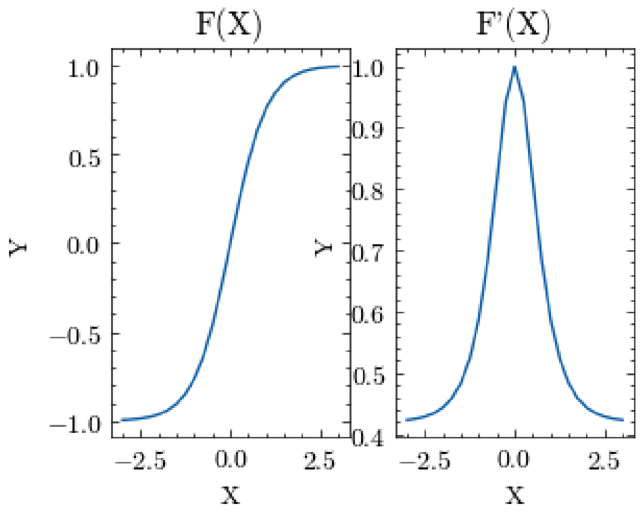
Tanh Activation Function Gradient

Since gradient descent relies on knowing the gradient of our activation function, let's derivate the gradient of the tanh function.

$$\begin{aligned}
\sigma'(z) &= \frac{\partial}{\partial z}[\frac{e^z - e^{-z}}{e^z + e^{-z}}] \\
&= \frac{(e^z + e^{-z})\frac{\partial}{\partial z}[e^z - e^{-z}] - (e^z - e^{-z})\frac{\partial}{\partial z}[e^z + e^{-z}]}{(e^z + e^{-z})^2} \\
&= \frac{(e^z + e^{-z})(e^z + e^{-z}) - (e^z - e^{-z})(e^z - e^{-z})}{(e^z + e^{-z})^2} \\
&= \frac{(e^z + e^{-z})^2 - (e^z - e^{-z})^2}{(e^z + e^{-z})^2} \\
&= \frac{(e^z + e^{-z})^2}{(e^z + e^{-z})^2} - \frac{(e^z - e^{-z})^2}{(e^z + e^{-z})^2} \\
&= 1 - [\sigma(z)]^2
\end{aligned}$$

Now that we have derived the gradient of the Tanh function, let's create the class for the Tanh activation function.

```
class Tanh(Activation):
    def __init__(self):
        tanh = lambda x: np.tanh(x)
        tanh_prime = lambda x: 1 - np.tanh(x) ** 2
        super().__init__(tanh, tanh_prime)


Tanh().plot(-3, 3)
```



0.7.11 Optimizer

Our optimization algorithm will be Gradient Descent, allowing us to determine how to update the parameters in the next iteration. $X\_\{n+1\} = X\_n - lr * \frac{\partial}{\partial X} f(X\_n)$.

Let's create a class that updates the weight matrix and the bias vector using the Gradient Descent equation.

```
class GradientDescentOptimizier:
    def __init__(self, learning_rate):
        self.learning_rate = learning_rate

    def backward(self, weights, weights_gradient, bias, output_gradient):
        weights -= self.learning_rate * weights_gradient
        bias -= self.learning_rate * output_gradient

        return weights, bias
```

0.7.12 Graphing Functions

This Notebook will create many visualizations of the neural network during its training phase.

`create_scatter_and_3d_plot()` creates a 2 column graph for the Mean Squared Error graph on the left and a 3D graph on the right.

`create_3d_and_3d_plot()` creates a 2 column graph with two 3D graphs.

`plot_3d_predictions()` plots the neural network's current preditions and the expected output of the neural network.

`plot_layer_loss_landscape()` plots how close one layer's current weights are from the optimal weights by seeing how the total mean squared error changes if the weights were shifted a little.

```python
import copy


def create_scatter_and_3d_plot():
    fig, ax = plt.subplots(1, 3, figsize=(16 / 9.0 * 4, 4 * 1))
    fig.suptitle("Neural Network Predictions")

    ax[0].set_xlabel("Epoch", fontweight="normal")
    ax[0].set_ylabel("Error", fontweight="normal")
    ax[0].set_title("Mean Squared Error")

    ax[1].axis("off")
    ax[2].axis("off")

    ax[2] = fig.add_subplot(1, 2, 2, projection="3d")
    ax[2].set_xlabel("X")
    ax[2].set_ylabel("Y")
    ax[2].set_zlabel("Z")
    ax[2].set_title("Function Approximation")
    ax[2].view_init(20, -35)
    ax[2].set_zlim(-1, 1)
    ax[2].axis("equal")

    camera = Camera(fig)
    return ax[0], ax[2], camera


def create_3d_and_3d_plot():
    fig, ax = plt.subplots(
        1, 2, figsize=(16 / 9.0 * 4, 4 * 1), subplot_kw={"projection": "3d"}
    )
    fig.suptitle("Neural Network Loss Landscape")

    ax[0].set_xlabel("W3_1")
    ax[0].set_ylabel("W3_2")
    ax[0].set_zlabel("MSE")
    ax[0].set_title("Mean Squared Error")
    ax[0].view_init(20, -35)
    ax[0].set_zlim(-1, 1)
    ax[0].axis("equal")

    ax[1].set_xlabel("X")
    ax[1].set_ylabel("Y")
    ax[1].set_zlabel("Z")
    ax[1].set_title("Function Approximation")
    ax[1].view_init(20, -35)
    ax[1].set_zlim(-1, 1)
    ax[1].axis("equal")

    camera = Camera(fig)
    return ax[0], ax[1], camera


def plot_3d_predictions(ax, X, Y, Z, predictions, dims):
    # Plot Neural Network Function Approximation
    # Ground truth
    ground_truth_legend = ax.plot_surface(
        X, Y, Z, color="red", alpha=0.5, label="Ground Truth"
    )

    # Neural Network Predictions
    predictions_legend = ax.scatter(
        X,
        Y,
        predictions.reshape((dims, dims)),
        color="blue",
        alpha=0.2,
        label="Prediction",
    )
    ax.plot_surface(
        X,
        Y,
        predictions.reshape((dims, dims)),
        color="blue",
        alpha=0.3,
    )
    ax.legend(
        (ground_truth_legend, predictions_legend),
        ("Ground Truth", "Predictions"),
        loc="upper left",
    )


def plot_layer_loss_landscape(
    ax0,
    network,
    target_layer_idx,
    features,
    labels,
    w1_min,
    w1_max,
    w2_min,
    w2_max,
    loss_dims,
):
    # current target layer weights
    target_layer_idx = target_layer_idx % len(network)

    w1 = network[target_layer_idx].weights[0][0]
    w2 = network[target_layer_idx].weights[0][1]
    curr_error = 0
    for x, y in zip(features, labels):
        output = x
        for layer in network:
            output = layer.forward(output)

        curr_error += mse(y, output)
    curr_error /= labels.size
    ax0.scatter([w1], [w2], [curr_error], color="red", alpha=0.4)

    target_layer = copy.deepcopy(network[target_layer_idx])
    w1_range = np.linspace(w1_min, w1_max, loss_dims)
    w2_range = np.linspace(w2_min, w2_max, loss_dims)
    w1_range, w2_range = np.meshgrid(w1_range, w2_range)
    w_range = np.stack((w1_range.flatten(), w2_range.flatten()), axis=1)

    error_range = np.array([])

    for target_layer_weight in w_range:
```

0.7.13 Training the model

Let's tie everything together to train the neural network. In each epoch, we will do the following:

1. Pass the training data into our model to get the model's predictions
2. Calculate the loss from the model's predictions and the expected value
3. Use the loss to run the optimizer to update the weights and biases
4. Call the visualization functions to visualize the training process

```
def fit(
    network,
    features,
    labels,
    X,
    Y,
    Z,
    preds_dims,
    epochs,
    optimizer,
    mse_plot_filename,
    loss_landscape_plot_filename,
):
    mse_idx = np.arange(1, epochs + 1)
    errors = np.full(epochs, -1)
    mse_ax, predictions_ax1, camera1 = create_scatter_and_3d_plot()
    loss_landscape_ax, predictions_ax2, camera2 = create_3d_and_3d_plot()

    network_len = len(network)

    for idx in range(epochs):
        error = 0
        predictions = np.array([])

        for x, y in zip(features, labels):
            # Forward Propagation
            output = x
            for layer in network:
                output = layer.forward(output)

            predictions = np.append(predictions, output)

            # Store Error
            # no need to convert to numpy cpu, since both are tensors on device
            error += mse(y, output)

            # Backpropagation
            grad = mse_prime(y, output)
            for layer in reversed(network):
                grad = layer.backward(grad, optimizer)

        error /= len(X)

        if show_epoch(idx):
            print(f"epoch: {idx}, MSE: {error}")

            # Plot MSE
            errors[idx] = error
            visible_mse = errors != -1
            plot_mse_and_predictions(
                mse_ax,
                predictions_ax1,
                idx,
                visible_mse,
                mse_idx,
                errors,
                X,
                Y,
                Z,
                predictions,
                preds_dims,
            )

            # plot the loss landscape of the second to last layer
            # a 3D plot can be made because it's only 2 neurons
            plot_loss_landscape_and_predictions(
                loss_landscape_ax,
                predictions_ax2,
                network,
                -2,
                features,
                labels,
                X,
                Y,
                Z,
                predictions,
                preds_dims,
            )

            camera1.snap()
            camera2.snap()

    animation1 = camera1.animate()
    animation1.save(mse_plot_filename, writer="pillow")

    animation2 = camera2.animate()
    animation2.save(loss_landscape_plot_filename, writer="pillow")
    plt.show()
```

The model can be visualized with the following:

Our model consists of 3 layers with the Tanh() activation function after each layer.

Layer 1: - Input Dimensions: 2 - Output Dimensions: 12

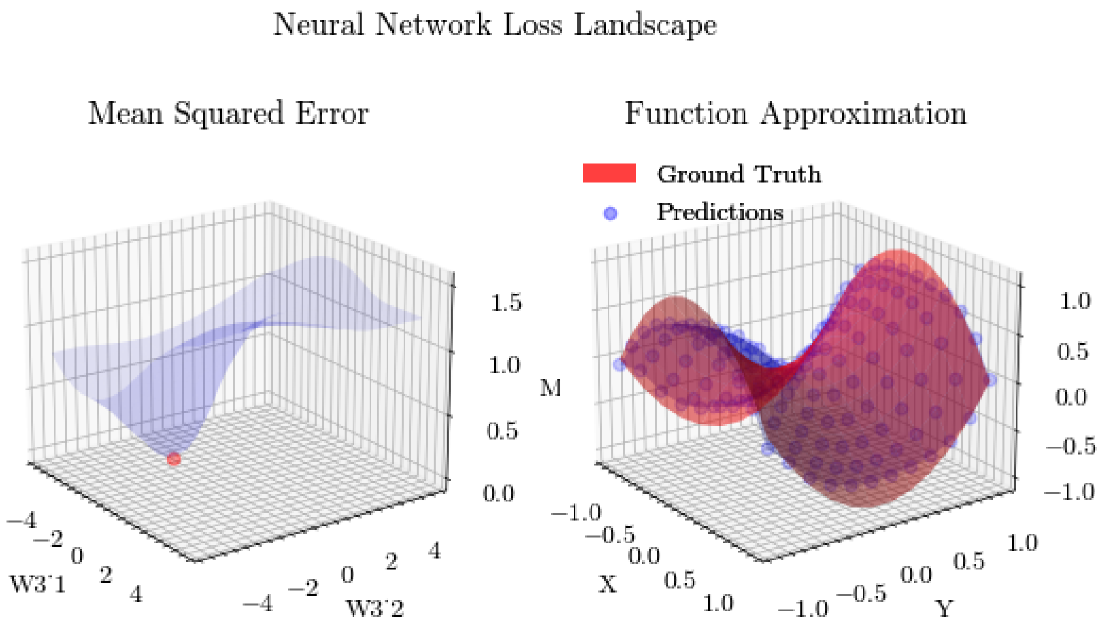
Layer 2: - Input Dimensions: 12 - Output Dimensions: 2

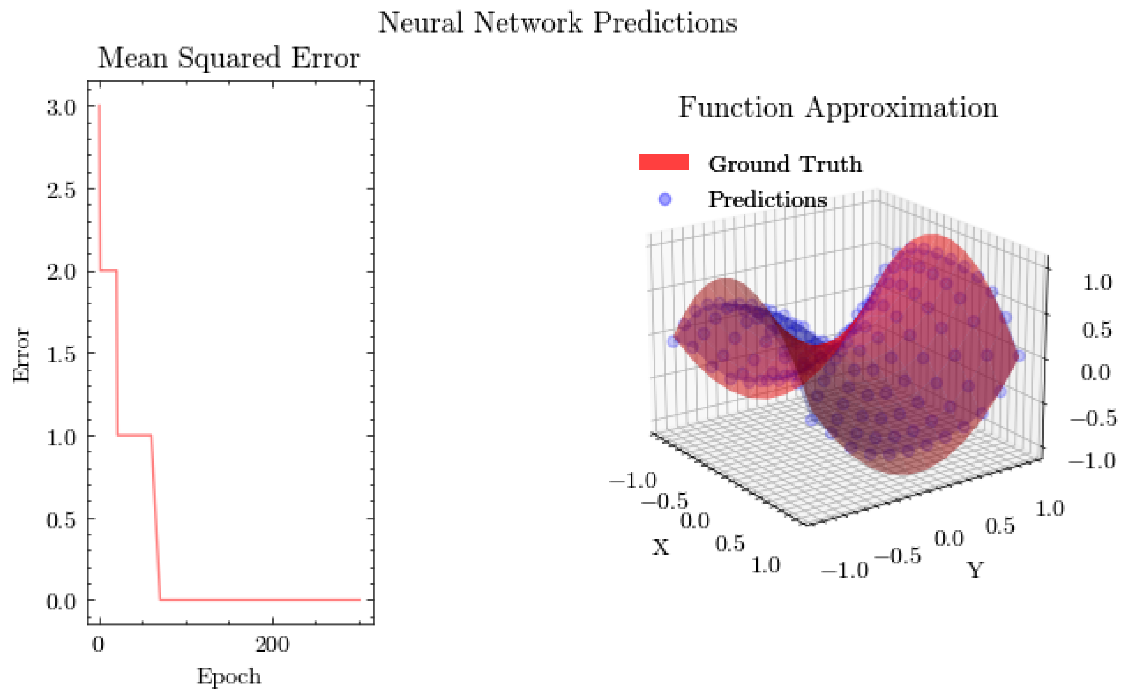
Layer 3: - Input Dimensions: 2 - Output Dimensions: 1

```
model = [Dense(2, 12), Tanh(), Dense(12, 2), Tanh(), Dense(2, 1), Tanh()]
```

Let's train our model by passing our model and optimizer to our training method

```
epochs = 301
learning_rate = 0.005
optimizer = GradientDescentOptimizier(learning_rate)

mse_plot_filename = "neural_network.gif"
loss_landscape_plot_filename = "neural_network_loss_landscape.gif"
fit(
    model,
    features,
    labels,
    X,
    Y,
    Z,
    dims,
    epochs,
    optimizer,
    mse_plot_filename,
    loss_landscape_plot_filename,
)
```





0.7.14 Output GIF

In this visualization, we see the predictions fit the ground truth. The neural network was able to find the optimal parameters to fit this function. Now think about the applications of this. Given input data about people's shopping habits, we can predict things to recommend to them. We can recommend a social media post to show them or a show to watch next. We can pass data to neural networks and it will uncover patterns from input data and find patterns.

The visualization below shows that backpropagation finds the optimal weights for the neural network. On the left graph, the red dot shows the current values of the weight matrix in the last layer of the neural network. The z axis is the mean squared error loss. If the weights weren't at the current value, the loss wouldn't be at a minima, meaning that backpropagation in fact does update the weights to the most optimal (local extrema) value and allows the network to converge.

0.7.15 Pytorch Implementation

Machine Learning libraries, such as PyTorch, provide utilities to easily train and test neural networks on all types of optimized hardware. Now we will implement the same network in PyTorch.

```
import torch
import torch.nn as nn
import torch.nn.functional as F

torch.manual_seed(0)
```

0.7.16 PyTorch nn.Module

We represent our neural network by creating a subclass of the `nn.Module` PyTorch class that defines all of the layers in the network and how data flows through the network. The `forward()` method is the forward propagation of our neural forward. Notice that we don't need to specify anything for the backpropagation process. PyTorch takes care of this for us using their auto-differentiation support. We just need to import an optimizer class, like the PyTorch provided gradient descent class, and pass in our model's parameters. This is the beauty of using machine learning libraries.

```
class TorchNet(nn.Module):
    def __init__(self):
        super(TorchNet, self).__init__()

        # define the layers
        self.fc1 = nn.Linear(2, 14)
        self.fc2 = nn.Linear(14, 2)
        self.fc3 = nn.Linear(2, 1)

    def forward(self, x):
        # pass the result of the previous layer to the next layer
        x = F.tanh(self.fc1(x))
        x = F.tanh(self.fc2(x))
        return F.tanh(self.fc3(x))
```

0.7.17 PyTorch Training

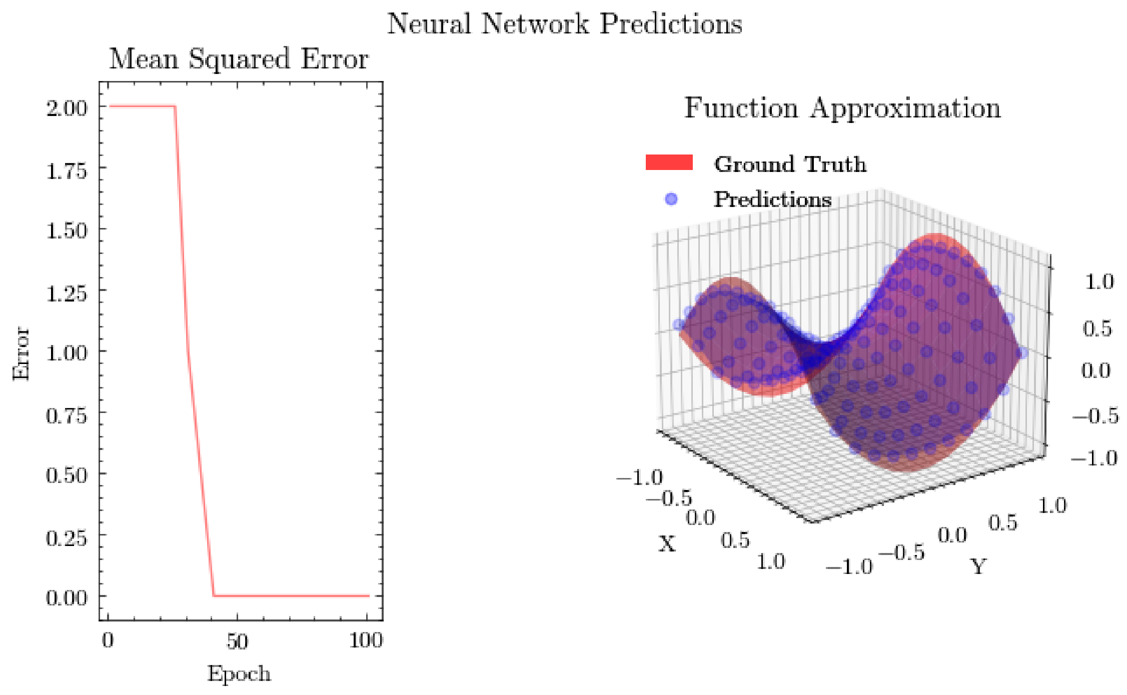
Similar to our own implementation, let's use our model to define our training process. In each epoch, we will do the following:

1. Pass the training data into our model to get the model's predictions
2. Calculate the loss from the model's predictions and the expected value
3. Use the loss to run the optimizer to update the weights and biases
4. Call the visualization functions to visualize the training process

```
def torch_fit(
    model, features, labels, X, Y, Z, dims, epochs, optimizer, output_filename
):
    mse_idx = np.arange(1, epochs + 1)
    errors = np.full(epochs, -1)
    mse_ax, predictions_ax1, camera1 = create_scatter_and_3d_plot()

    loss_fn = nn.MSELoss()

    for idx in range(epochs):
        error = 0
        predictions = np.array([])

        for x, y in zip(features, labels):
            # Forward Propagation
            output = model(x)

            output_np = output.detach().cpu().numpy()
            predictions = np.append(predictions, output_np)

            # Store Error
            loss = loss_fn(output, y)

            error += loss.detach().cpu().numpy()

            # Backpropagation
            optimizer.zero_grad()
            loss.backward()
            optimizer.step()

        error /= len(X)

        if show_epoch(idx):
            print(f"epoch: {idx}, MSE: {error}")

            # Plot MSE
            errors[idx] = error
            visible_mse = errors != -1

            plot_mse_and_predictions(
                mse_ax,
                predictions_ax1,
                idx,
                visible_mse,
                mse_idx,
                errors,
                X,
                Y,
                Z,
                predictions,
                dims,
            )

            camera1.snap()

    animation1 = camera1.animate()
    animation1.save(output_filename, writer="pillow")
    plt.show()
```

Let's call the training method and pass in the model, training data, and optimizer.

```
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
torch_model = TorchNet().to(device)

# the inputs and outputs for PyTorch must be tensors
features_tensor = torch.tensor(features, device=device, dtype=torch.float32).squeeze(-1)
labels_tensor = torch.tensor(labels, device=device, dtype=torch.float32).squeeze(-1)

epochs = 101
learning_rate = 0.005
optimizer = torch.optim.SGD(torch_model.parameters(), lr=learning_rate, momentum=0.0)

output_filename_pytorch = "neural_network_pytorch.gif"
torch_fit(
    torch_model,
    features_tensor,
    labels_tensor,
    X,
    Y,
    Z,
    dims,
    epochs,
    optimizer,
    output_filename_pytorch,
)
```


Neural Network Predictions
Mean Squared Error
Error
Epoch
Function Approximation
Ground Truth
Predictions
X
Y