lab2

March 19, 2025

0.1 Gradient Descent Extensions: Momentum and Adam - Radosław Kawa

0.1.1 0. Methods

[3]:
```
import numpy as np
from abc import ABC, abstractmethod

class Problem(ABC):
    @abstractmethod
    def __call__(self, x: np.ndarray) -> float:
        """Compute the function value at point x."""
        raise NotImplementedError

    @abstractmethod
    def grad(self, x: np.ndarray) -> np.ndarray:
        """Compute the gradient at point x."""
        raise NotImplementedError

class Sphere(Problem):
    def __call__(self, x: np.ndarray) -> float:
        return np.sum(x**2)

    def grad(self, x: np.ndarray) -> np.ndarray:
        return 2 * x

class Rosenbrock(Problem):
    def __call__(self, x: np.ndarray) -> float:
        return np.sum(100.0 * (x[1:] - x[:-1]**2)**2 + (1 - x[:-1])**2)

    def grad(self, x: np.ndarray) -> np.ndarray:
        grad = np.zeros_like(x)
        n = x.size
        grad[0] = -400 * x[0] * (x[1] - x[0]**2) - 2 * (1 - x[0])
        for i in range(1, n - 1):
            grad[i] = 200 * (x[i] - x[i-1]**2) - 400 * x[i] * (x[i+1] -␣
↪x[i]**2) - 2 * (1 - x[i])
        grad[-1] = 200 * (x[-1] - x[-2]**2)
        return grad
```

```python
class Rastrigin(Problem):
    def __call__(self, x: np.ndarray) -> float:
        A = 10
        n = x.size
        return A * n + np.sum(x**2 - A * np.cos(2 * np.pi * x))

    def grad(self, x: np.ndarray) -> np.ndarray:
        A = 10
        return 2 * x + 2 * np.pi * A * np.sin(2 * np.pi * x)
```

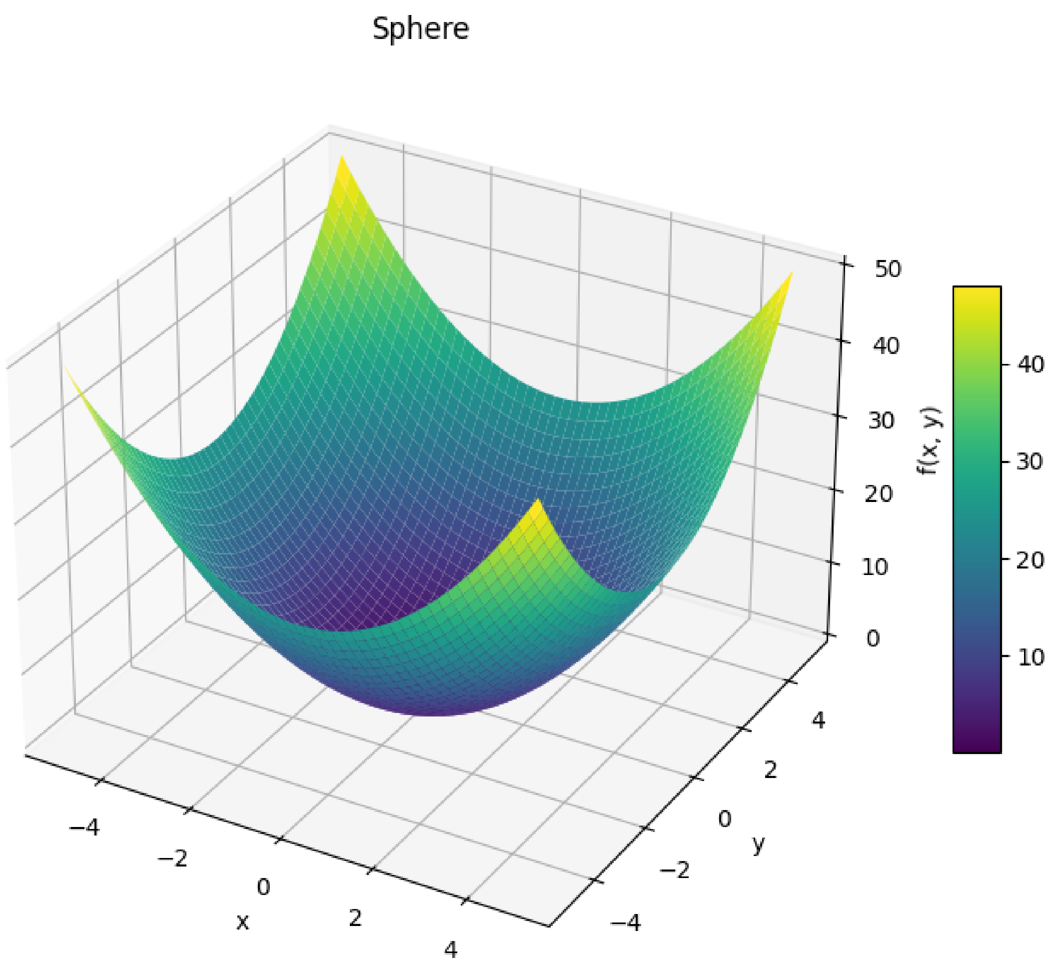
[4]:
```python
import matplotlib.pyplot as plt
import plotly.graph_objects as go

def prepare_mesh_grid(
    problem: Problem,
    bounds: tuple[float, float] = (-5.0, 5.0),
    grid_size: int = 50,
) -> tuple[np.ndarray, np.ndarray, np.ndarray, np.ndarray, np.ndarray]:
    x_vals = np.linspace(bounds[0], bounds[1], grid_size)
    y_vals = np.linspace(bounds[0], bounds[1], grid_size)
    X, Y = np.meshgrid(x_vals, y_vals)

    Z = np.zeros_like(X)
    for i in range(grid_size):
        for j in range(grid_size):
            xy = np.array([X[i, j], Y[i, j]])
            Z[i, j] = problem(xy)

    return X, Y, Z, x_vals, y_vals


def plot_3d_surface(
    problem: Problem,
    grid_size: int = 50,
):
    X, Y, Z, _, _ = prepare_mesh_grid(problem=problem, grid_size=grid_size)

    fig = plt.figure(figsize=(8, 6))
    ax = fig.add_subplot(111, projection="3d")
    surf = ax.plot_surface(X, Y, Z, cmap="viridis", edgecolor="none")

    ax.set_title(problem.__class__.__name__)
    ax.set_xlabel("x")
    ax.set_ylabel("y")
    ax.set_zlabel("f(x, y)")
```

```
    fig.colorbar(surf, shrink=0.5, aspect=10)
    plt.tight_layout()
    plt.show()

def plot_contour_and_paths(
    problem: Problem,
    paths: list[np.ndarray],
    grid_size: int = 200,
    title: str = "",
):
    """
    Create an interactive contour plot of a 2D function and overlay multiple␣
 ↪optimization paths.

    Args:
        problem: An instance of a Problem class.
        paths: List of numpy arrays; each array is of shape (epochs, 2)␣
 ↪containing an optimization trajectory.
        title: Title for the plot.
    """
    _, _, Z, x_vals, y_vals = prepare_mesh_grid(problem, grid_size=grid_size)

    fig = go.Figure(
        data=go.Contour(
            x=x_vals,
            y=y_vals,
            z=Z,
            colorscale="Viridis",
            contours=dict(showlines=False),
            colorbar=dict(title="Function Value"),
        )
    )

    colors = ['red', 'blue', 'green', 'purple', 'orange', 'cyan', 'magenta',␣
 ↪'yellow', 'pink', 'brown']

    for idx, path in enumerate(paths):
        color_idx = idx % len(colors)
        fig.add_trace(
            go.Scatter(
                x=path[:, 0],
                y=path[:, 1],
                mode="lines+markers",
                marker=dict(size=4),
                line=dict(width=2, color=colors[color_idx]),
                name=f"Run {idx+1}",
                showlegend=True,
```

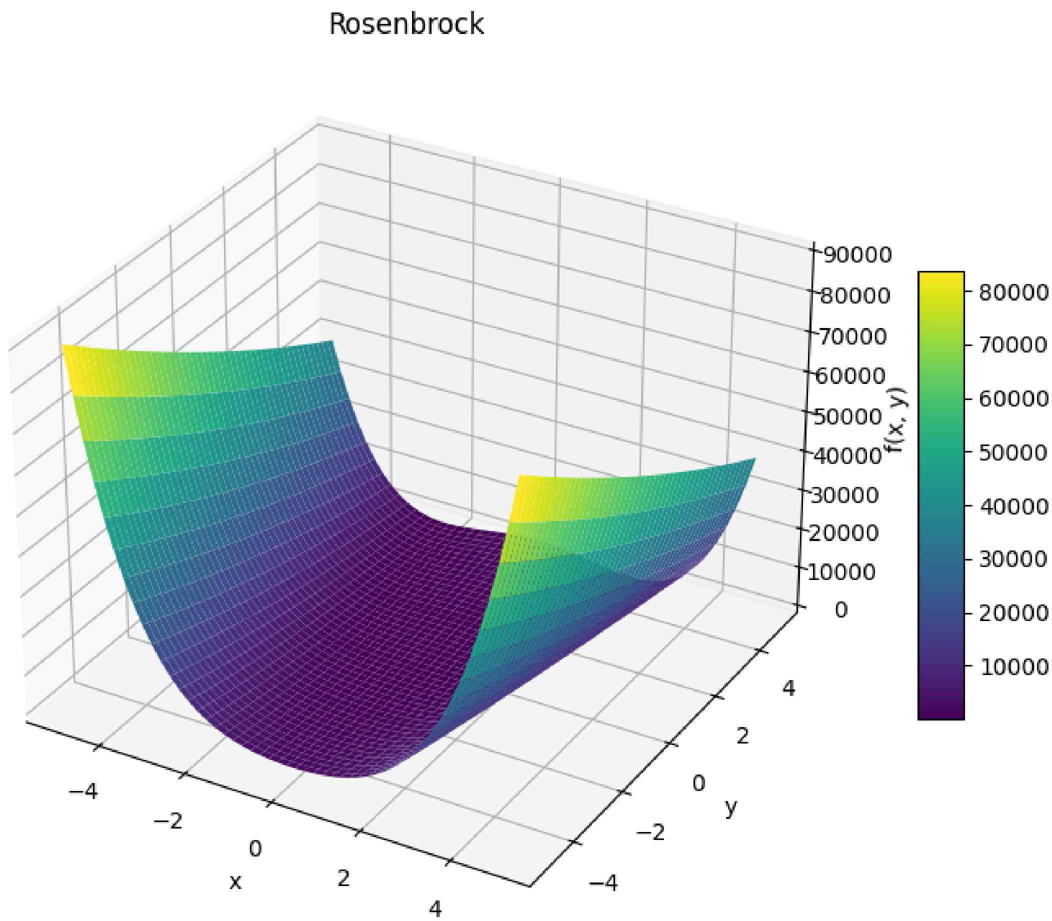
```
            )
        )

    fig.update_layout(
        title=title, xaxis_title="x", yaxis_title="y", width=800, height=700,
        legend=dict(orientation="h", yanchor="bottom", y=1.02, xanchor="right",␣
↪x=1)
    )

    fig.show()
```

0.1.2 1. Getting familiar with optimization test problems

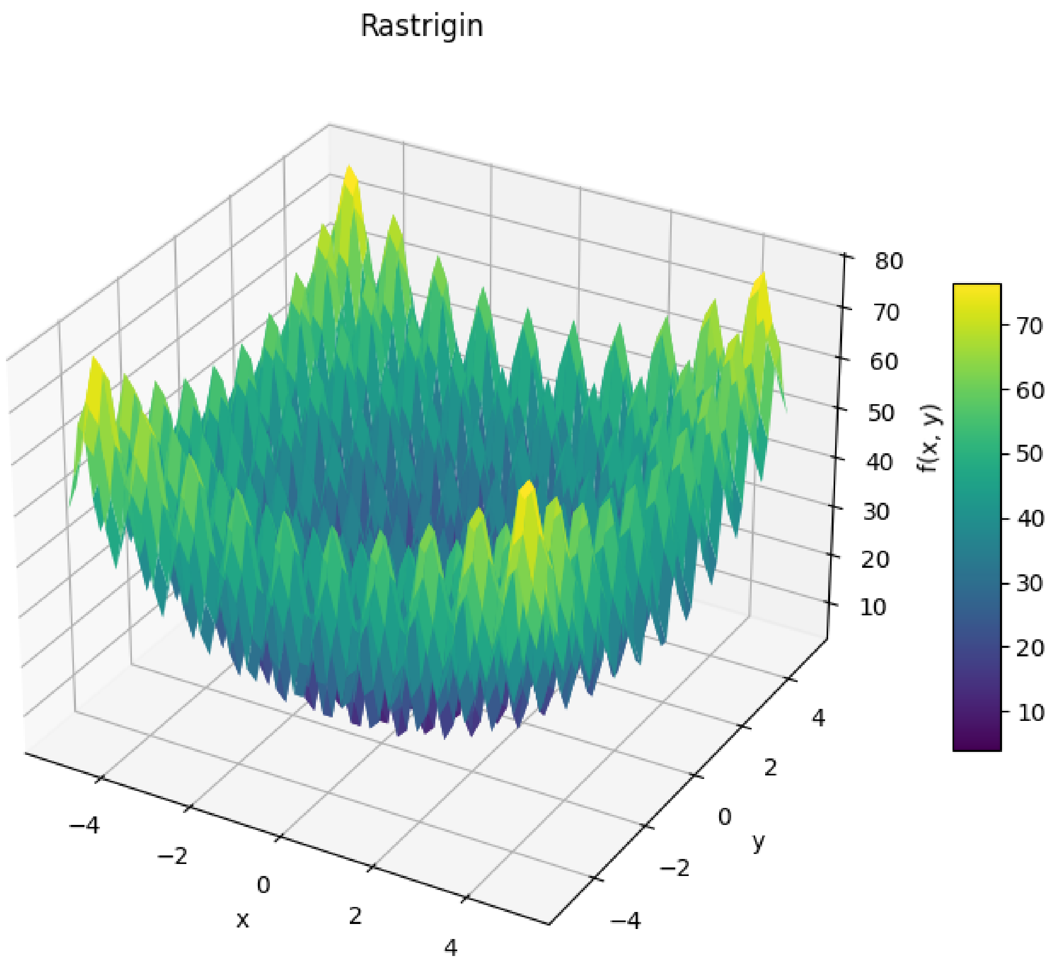
[84]:
```
plot_3d_surface(Sphere())
plot_contour_and_paths(Sphere(), [np.array([[0, 0]])], title="Sphere")
```



[85]:
```
plot_3d_surface(Rosenbrock())
plot_contour_and_paths(Rosenbrock(), [np.array([[0, 0]])], title="Rosenbrock")
```



[86]:
```
plot_3d_surface(Rastrigin())
plot_contour_and_paths(Rastrigin(), [np.array([[0,0]])], title="Rastrigin")
```



- Sphere function appears easiest to optimize because it is a convex function with a single global minimum at (0, 0).
- Rastrigin function appears hardestcto optimize because it has many local minima and is highly multimodal.
- Rosenbrock function is also hard to optimize because it is a non-convex function with a narrow, curved valley that leads to the global minimum at (1, 1).

0.1.3 2. Momentum method

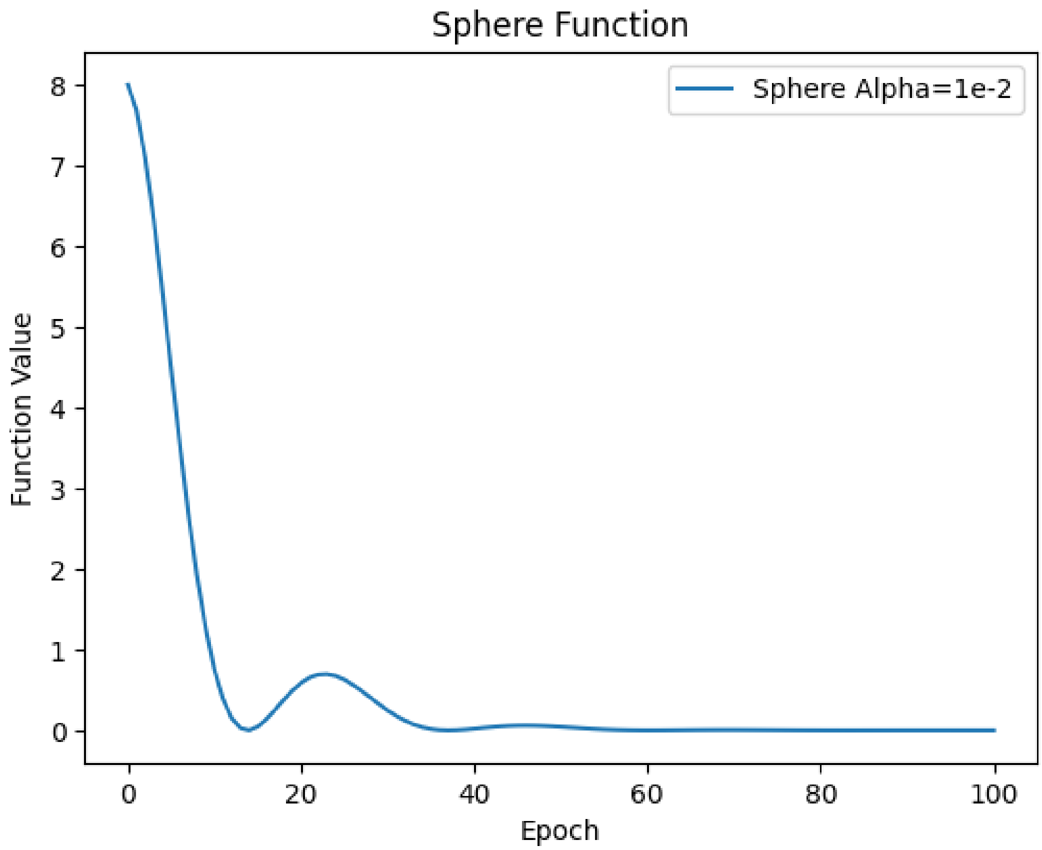
[102]:
```
def momentum(
    problem: Problem,
    initial_solution: np.ndarray,
    alpha: float,
    beta: float,
    number_of_epochs: int,
    clip_value: float = 1.0
):
```

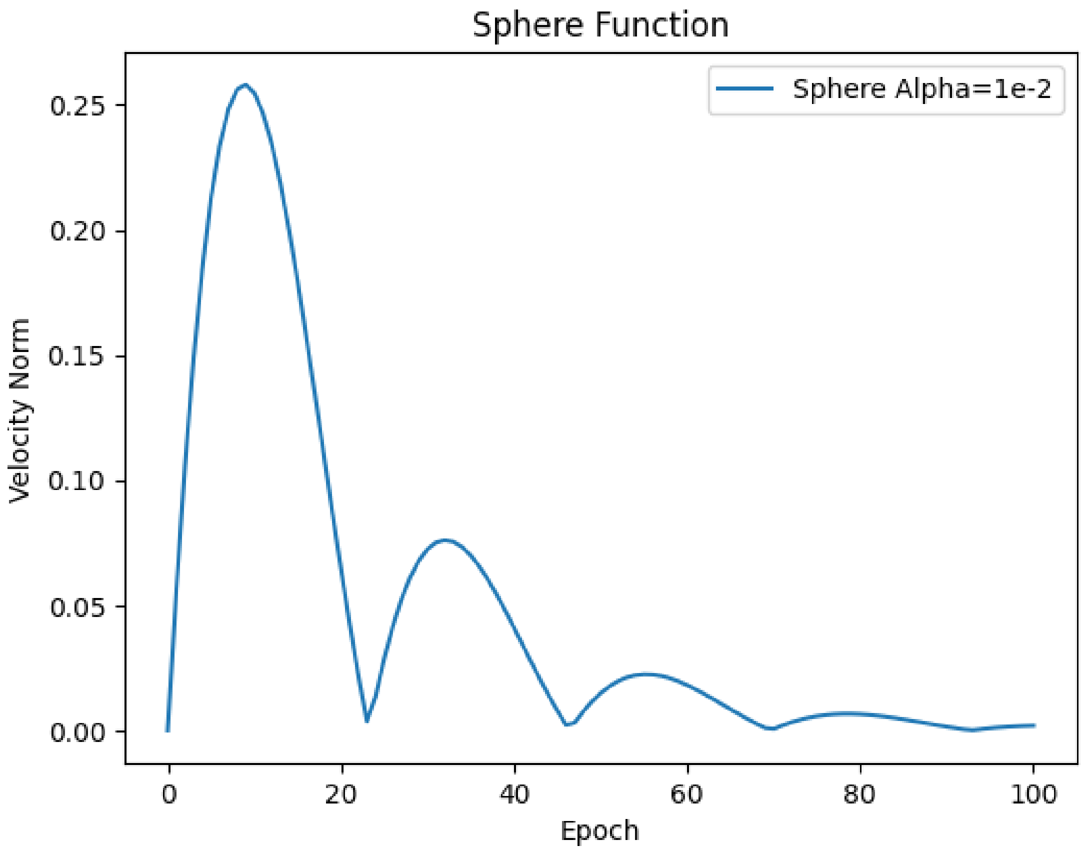
```
    x = initial_solution
    v = np.zeros_like(x)
    path = [x.copy()]
    velocities = [v.copy()]

    for _ in range(number_of_epochs):
        grad = problem.grad(x)
        # grad = np.clip(grad, -clip_value, clip_value)  # Clip the gradients
        v = beta * v + alpha * grad
        x = x - v
        path.append(x.copy())
        velocities.append(v.copy())

    return np.array(path), np.array(velocities)
```

0.1.4 3. Experiments with Momentum

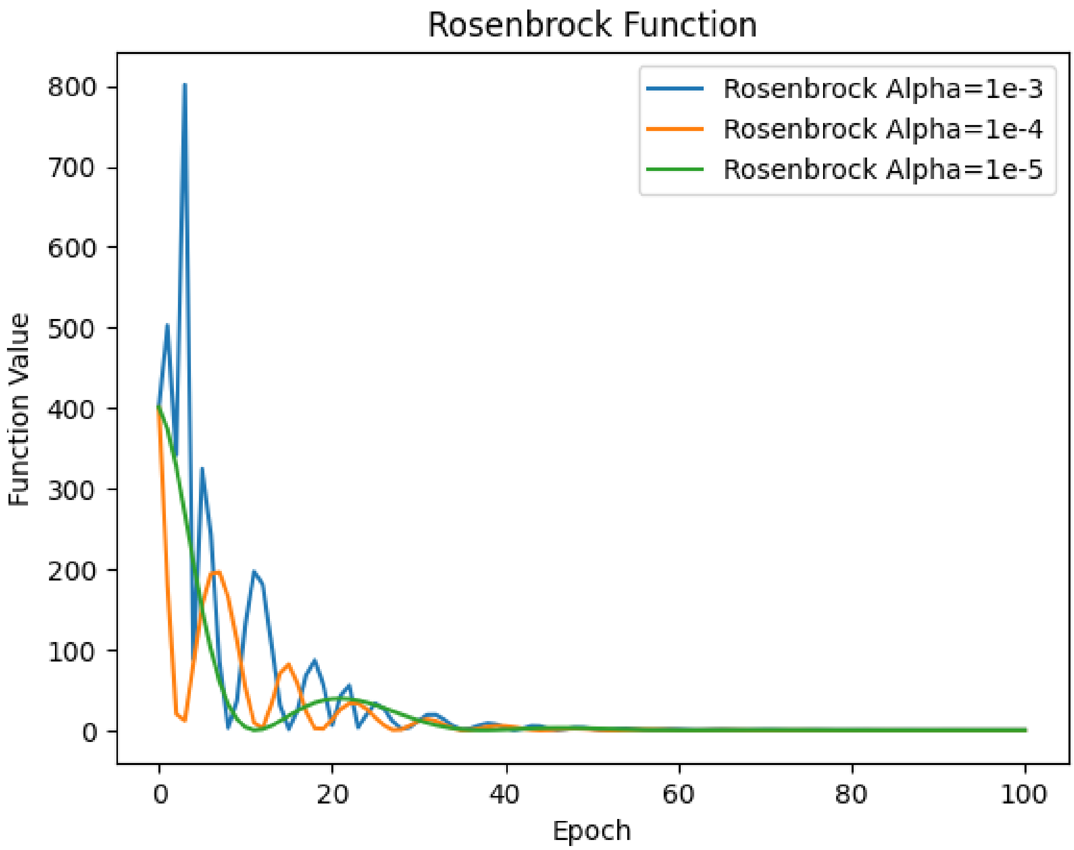
[103]:
```
def plot_function_values(problem, paths: list, legend_labels: list, title=str):
    for path, label in zip(paths, legend_labels):
        function_values = [problem(x) for x in path]
        plt.plot(function_values, label=label)
    plt.xlabel("Epoch")
    plt.ylabel("Function Value")
    plt.title(title)
    plt.legend()
    plt.show()

def plot_function_velocities(paths: list, legend_labels: list, title=str):
    for path, label in zip(paths, legend_labels):
        velocity_norms = [np.linalg.norm(v) for v in path]
        plt.plot(velocity_norms, label=label)
    plt.xlabel("Epoch")
    plt.ylabel("Velocity Norm")
    plt.title(title)
    plt.legend()
    plt.show()
```

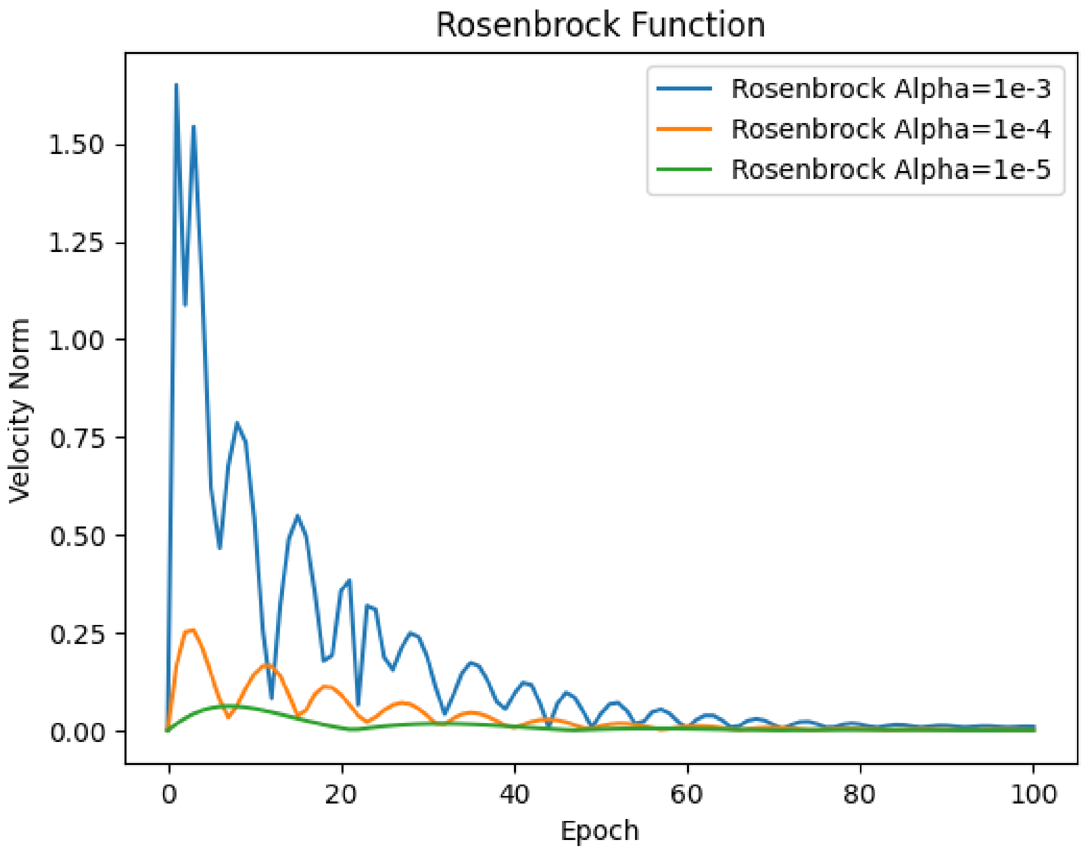
[104]:
```
initial_solution = np.array([2.0, 2.0])
beta = 0.9
number_of_epochs = 100

alpha = 1e-2
problem = Sphere()
path, velocities = momentum(problem, initial_solution, alpha, beta,␣
 ↪number_of_epochs)
plot_function_values(problem, [path], ["Sphere Alpha=1e-2"], "Sphere Function")
plot_function_velocities([velocities], ["Sphere Alpha=1e-2"], "Sphere Function")
```


Sphere Function
Sphere Alpha=1e-2
Function Value
Epoch
8
7
6
5
4
3
2
1
0
0
20
40
60
80
100

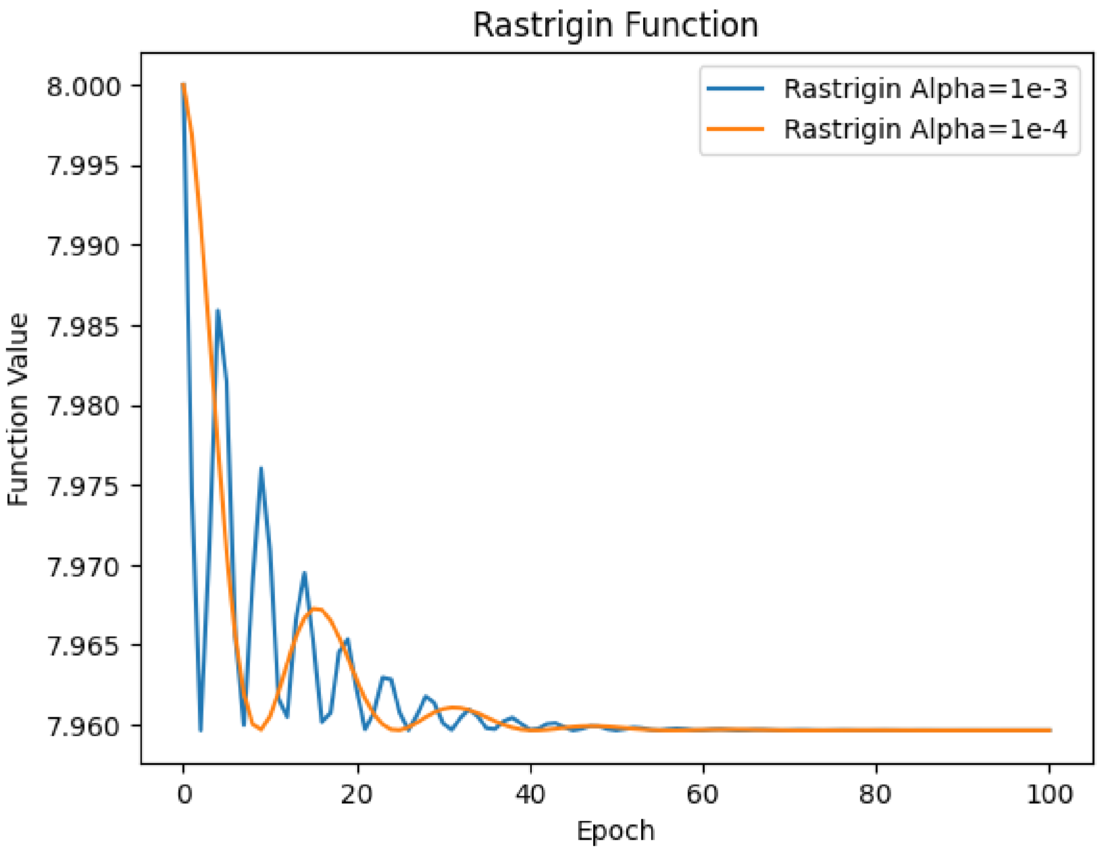


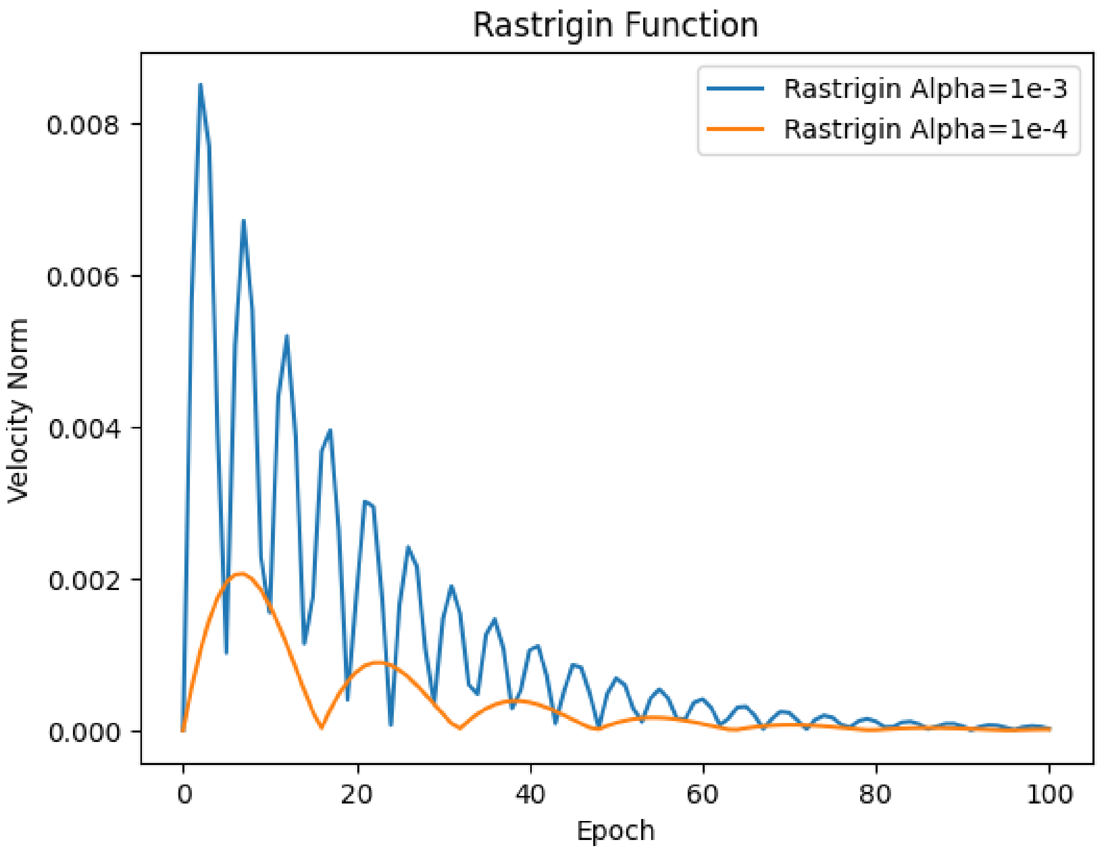
[107]:
```
paths, velocities = [], []

problem = Rosenbrock()
for alpha in [1e-3, 1e-4, 1e-5]:
    path, velocity = momentum(problem, initial_solution, alpha, beta,␣
 ↪number_of_epochs)
    paths.append(path)
    velocities.append(velocity)

plot_function_values(problem, paths, ["Rosenbrock Alpha=1e-3", "Rosenbrock␣
 ↪Alpha=1e-4", "Rosenbrock Alpha=1e-5"], "Rosenbrock Function")
plot_function_velocities(velocities, ["Rosenbrock Alpha=1e-3", "Rosenbrock␣
 ↪Alpha=1e-4", "Rosenbrock Alpha=1e-5"], "Rosenbrock Function")
```


Rosenbrock Function
Rosenbrock Alpha=1e-3
Rosenbrock Alpha=1e-4
Rosenbrock Alpha=1e-5
Function Value
Epoch
800
700
600
500
400
300
200
100
0
20
40
60
80
100



[108]:
```
paths, velocities = [], []

problem = Rastrigin()
for alpha in [1e-3, 1e-4]:
    path, velocity = momentum(problem, initial_solution, alpha, beta,␣
 ↪number_of_epochs)
    paths.append(path)
    velocities.append(velocity)

plot_function_values(problem, paths, ["Rastrigin Alpha=1e-3", "Rastrigin␣
 ↪Alpha=1e-4"], "Rastrigin Function")
plot_function_velocities(velocities, ["Rastrigin Alpha=1e-3", "Rastrigin␣
 ↪Alpha=1e-4"], "Rastrigin Function")
```


Rastrigin Function
Rastrigin Alpha=1e-3
Rastrigin Alpha=1e-4
8.000
7.995
7.990
7.985
7.980
7.975
7.970
7.965
7.960
Function Value
0
20
40
60
80
100
Epoch

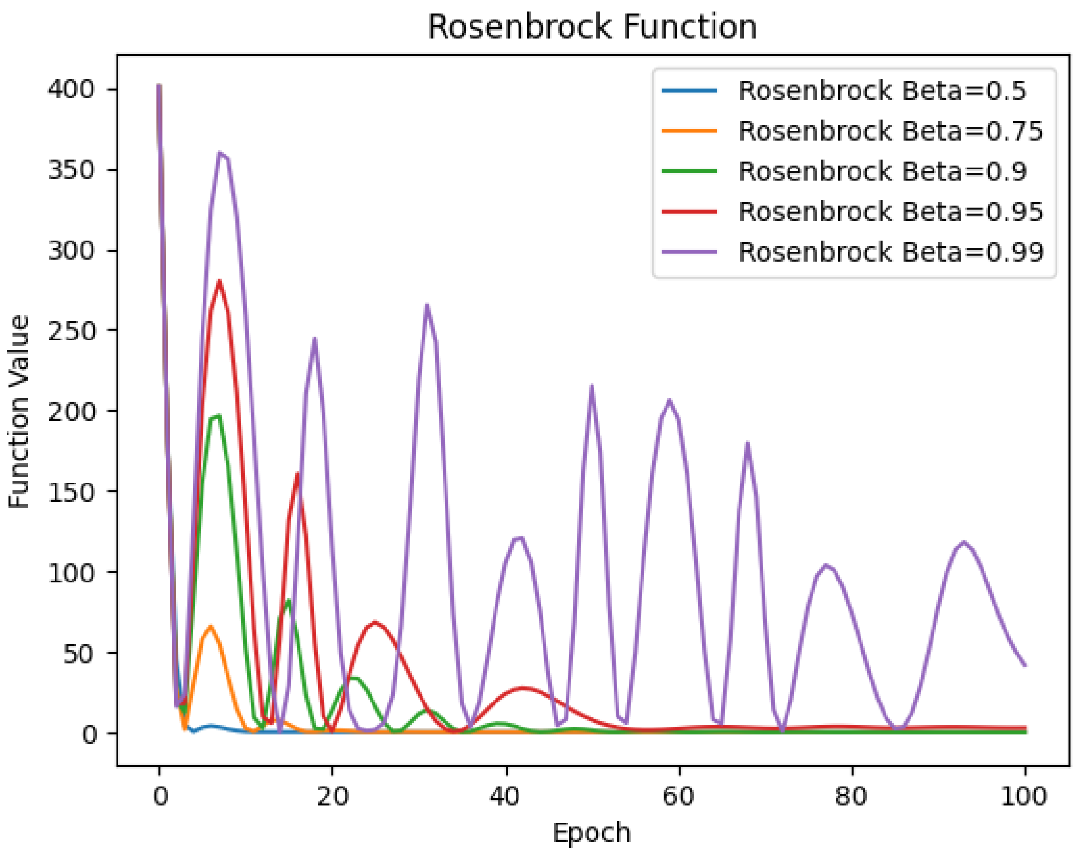


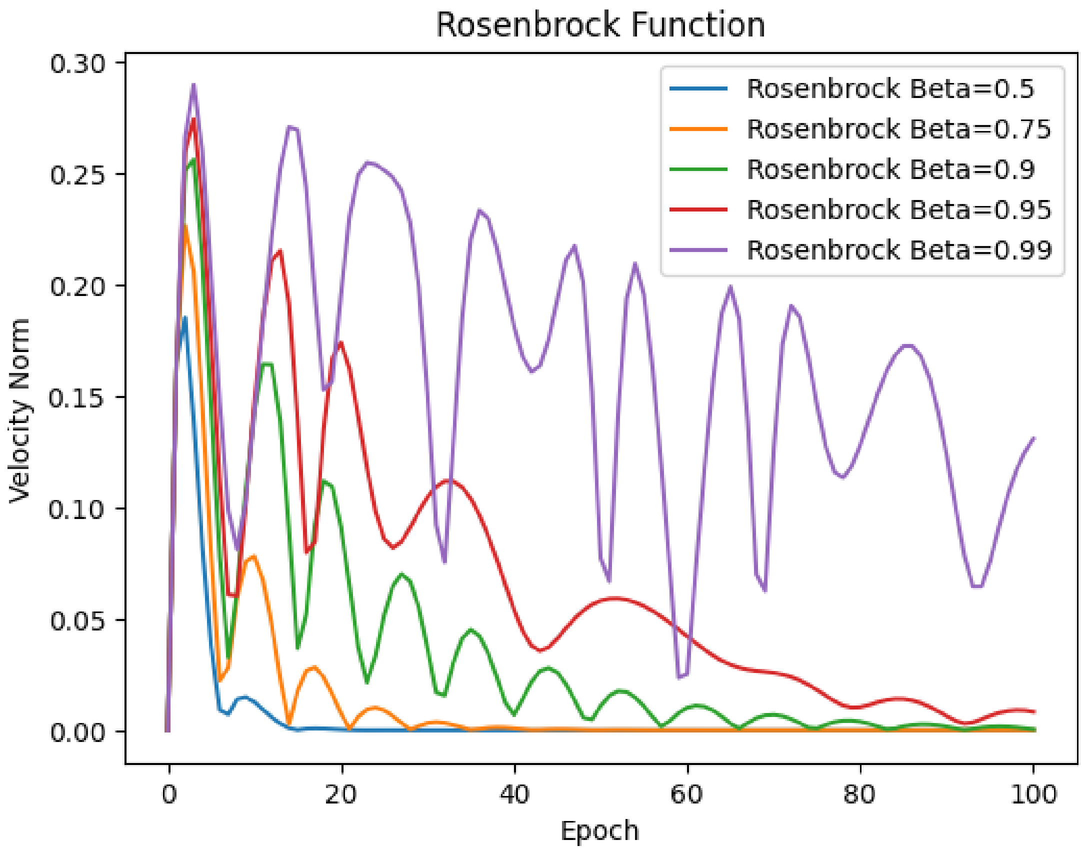
It seems that the velocity norm decreases as the optimization progresses. This is expected as the velocity is a moving average of the gradients, which should become smaller as the optimization converges. The velocity norm can be used as a proxy for the convergence speed, as it decreases as the optimization progresses.

0.1.5 4. Momentum Hyperparameters

[109]:
```
initial_solution = np.array([2.0, 2.0])
alpha = 1e-4
number_of_epochs = 100
betas = [0.5, 0.75, 0.9, 0.95, 0.99]

paths, velocities = [], []

problem = Rosenbrock()
for beta in betas:
    path, velocity = momentum(problem, initial_solution, alpha, beta,
 ↪number_of_epochs)
    paths.append(path)
    velocities.append(velocity)
```

```
plot_function_values(problem, paths, [f"Rosenbrock Beta={beta}" for beta in betas], "Rosenbrock Function")
plot_function_velocities(velocities, [f"Rosenbrock Beta={beta}" for beta in betas], "Rosenbrock Function")
```





Increasing makes the optimization faster, but it can also make the optimization unstable. If is too large, the optimization may oscillate around the minimum or even diverge. In practice, we need to find a good balance between the speed of convergence and stability.

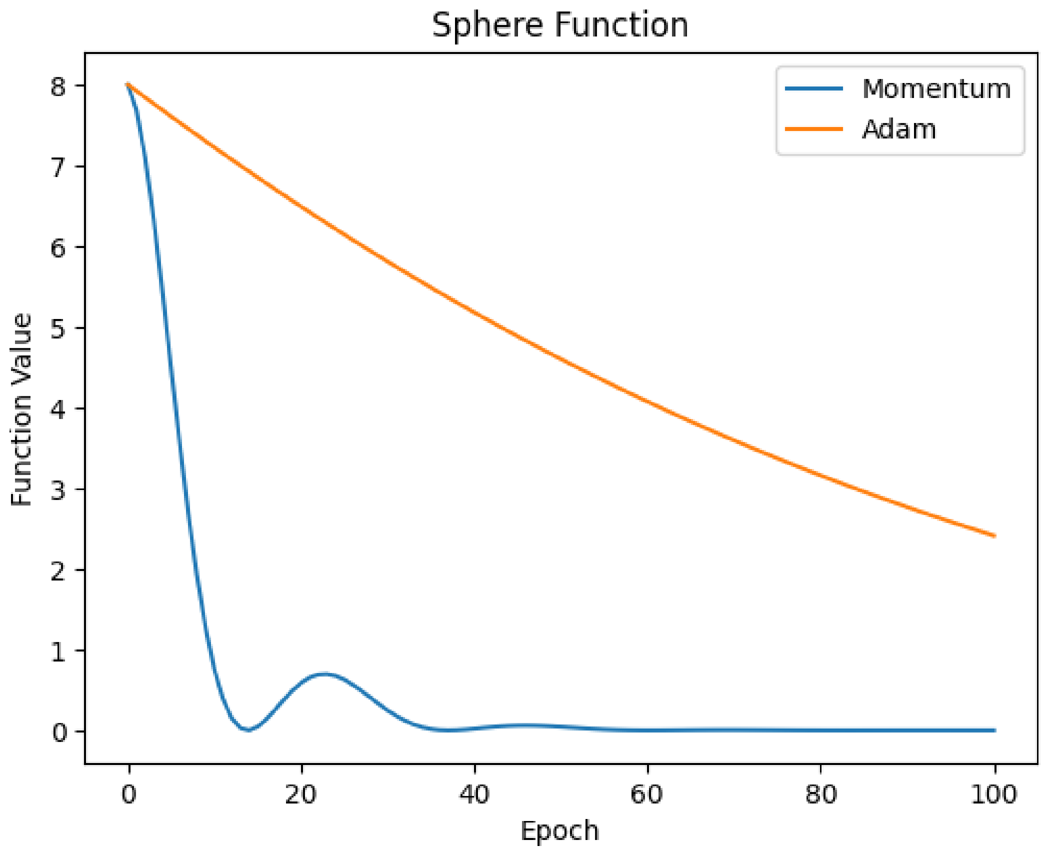
0.1.6 5. Adam

[110]:
```
def adam(
    problem: Problem,
    initial_solution: np.ndarray,
    alpha: float,
    beta1: float,
    beta2: float,
    number_of_epochs: int,
    epsilon: float = 1e-8
):
    x = initial_solution
    m = np.zeros_like(x)
    v = np.zeros_like(x)
    path = [x.copy()]
```

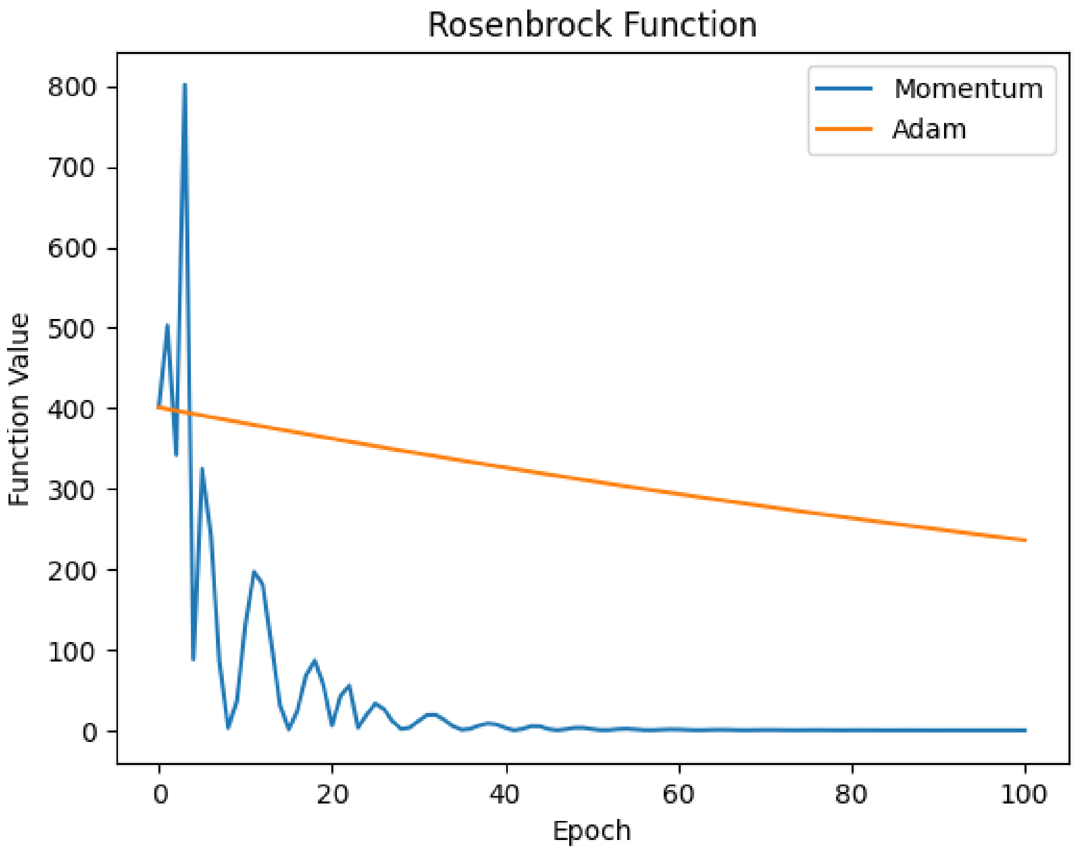
```
    for t in range(1, number_of_epochs + 1):
        g = problem.grad(x)
        m = beta1 * m + (1 - beta1) * g
        v = beta2 * v + (1 - beta2) * g**2
        m_hat = m / (1 - beta1**t)
        v_hat = v / (1 - beta2**t)
        x = x - alpha * m_hat / (np.sqrt(v_hat) + epsilon)
        path.append(x.copy())

    return np.array(path)
```

0.1.7 6. Comparing Adam with Momentum

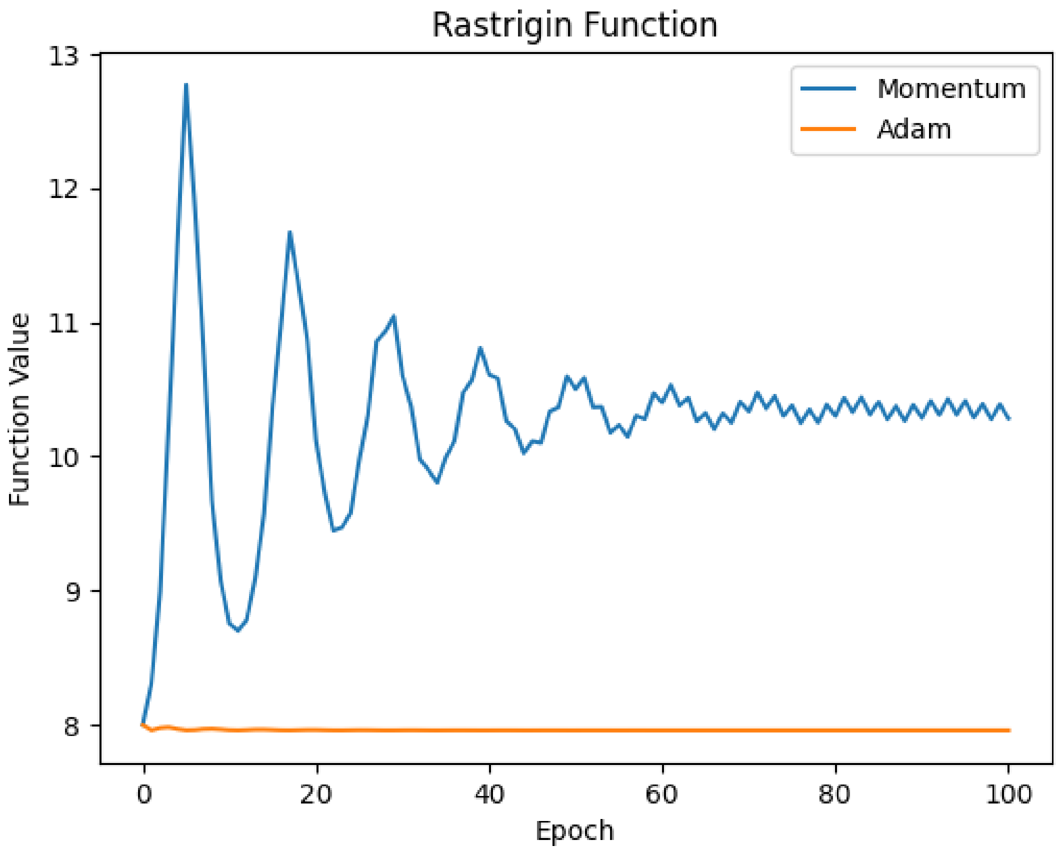
[128]:
```
initial_solution = np.array([2.0, 2.0])
number_of_epochs = 100

alpha = 0.01
beta = 0.9

beta1 = 0.9
beta2 = 0.999
epsilon = 1e-8

problem = Sphere()
path_momentum, _ = momentum(problem, initial_solution, alpha, beta,␣
 ↪number_of_epochs)
path_adam = adam(problem, initial_solution, alpha, beta1, beta2,␣
 ↪number_of_epochs, epsilon)

plot_contour_and_paths(problem, [path_momentum, path_adam], title="Sphere -␣
 ↪Momentum vs. Adam")
plot_function_values(problem,[path_momentum, path_adam], ["Momentum", "Adam"],␣
 ↪"Sphere Function")
```



[133]:
```
# I had to change alpha for momentum because of numerical instability (too␣
 ↪large numbers)
problem = Rosenbrock()
path_momentum, _ = momentum(problem, initial_solution, 0.001, beta,␣
 ↪number_of_epochs)
path_adam = adam(problem, initial_solution, 0.001, beta1, beta2,␣
 ↪number_of_epochs, epsilon)

plot_contour_and_paths(problem, [path_momentum, path_adam], title="Rosenbrock -␣
 ↪Momentum vs. Adam")
plot_function_values(problem,[path_momentum, path_adam], ["Momentum", "Adam"],␣
 ↪"Rosenbrock Function")
```



[130]:
```
problem = Rastrigin()
path_momentum, _ = momentum(problem, initial_solution, alpha, beta,␣
 ↪number_of_epochs)
path_adam = adam(problem, initial_solution, alpha, beta1, beta2,␣
 ↪number_of_epochs, epsilon)

plot_contour_and_paths(problem, [path_momentum, path_adam], title="Rastrigin -␣
 ↪Momentum vs. Adam")
plot_function_values(problem,[path_momentum, path_adam], ["Momentum", "Adam"],␣
 ↪"Rastrigin Function")
```



Rastrigin Function
Momentum
Adam
Function Value
Epoch
13
12
11
10
9
8
0
20
40
60
80
100