Variants of stochastic gradient-based optimization

In this assignment, we will implement Stochastic Gradient Optimization with different variants and try to find good hyperparameters for them.

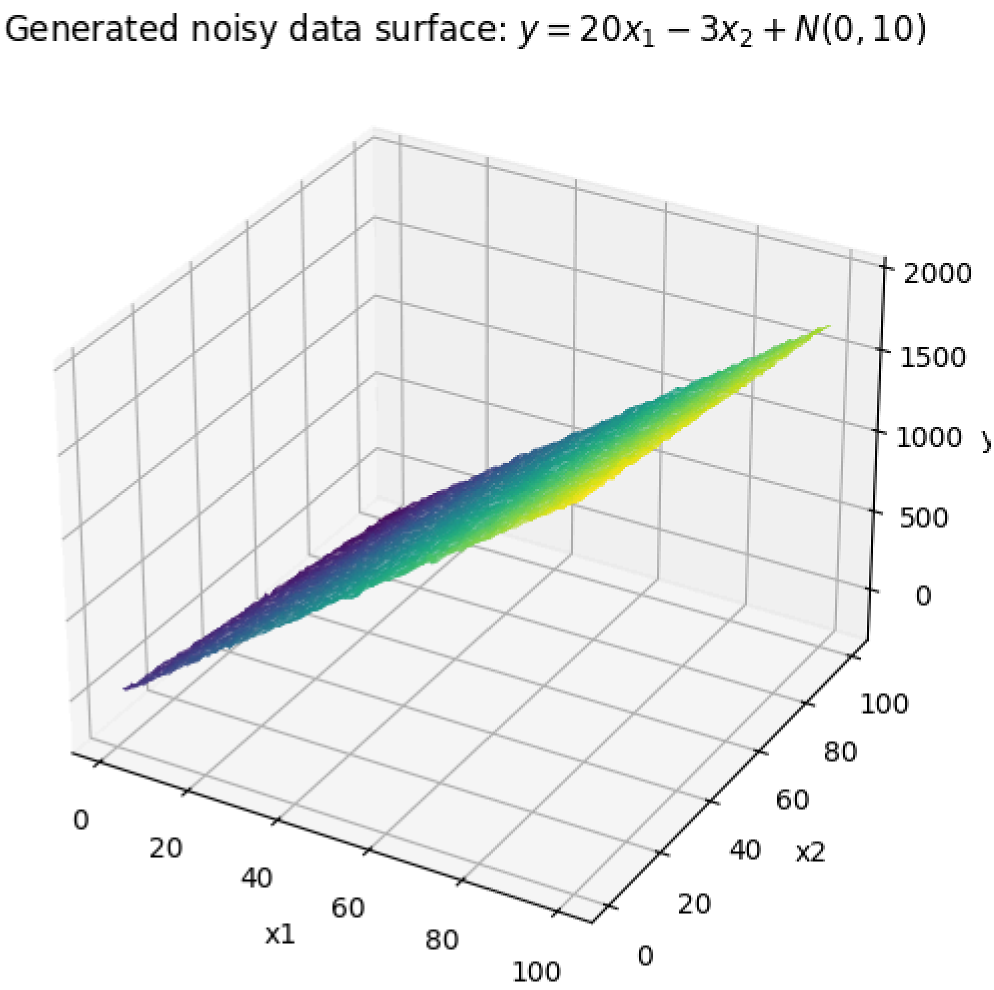
I will begin this notebook by setting the scene for what is to come by defining the data and the raw model that we will improve in the later stages. I will also use *MSE* as the loss function and its gradient.

1. Setting the scene

we begin like usual by just importing all of the dependencies and then defining the model parameters and values and then generating the 3D plot of the noisy data.

In [ ]:
```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
```

In [ ]:
```
np.random.seed(1)

# Parameters
N = 100
a10 = 20
a20 = -3
# Generate all combinations of (x1, x2) from 1 to N
X1, X2 = np.meshgrid(np.arange(1, N+1), np.arange(1, N+1))
X1 = X1.flatten()
X2 = X2.flatten()
X = np.column_stack((X1, X2))

# Generate noisy targets: y = 20*x1 - 3*x2 + noise
R = np.random.normal(0, 10, size=N*N)
Y = a10 * X1 + a20 * X2 + R

fig = plt.figure(figsize=(8, 6))
ax = fig.add_subplot(111, projection='3d')
ax.plot_trisurf(X[:, 0], X[:, 1], Y, cmap='viridis', linewidth=0.2)
ax.set_title("Generated noisy data surface: $y = 20x_1 - 3x_2 + N(0,10)$")
ax.set_xlabel("x1")
ax.set_ylabel("x2")
ax.set_zlabel("y")
plt.show()
```



we can then define the model, the loss function and its gradient.

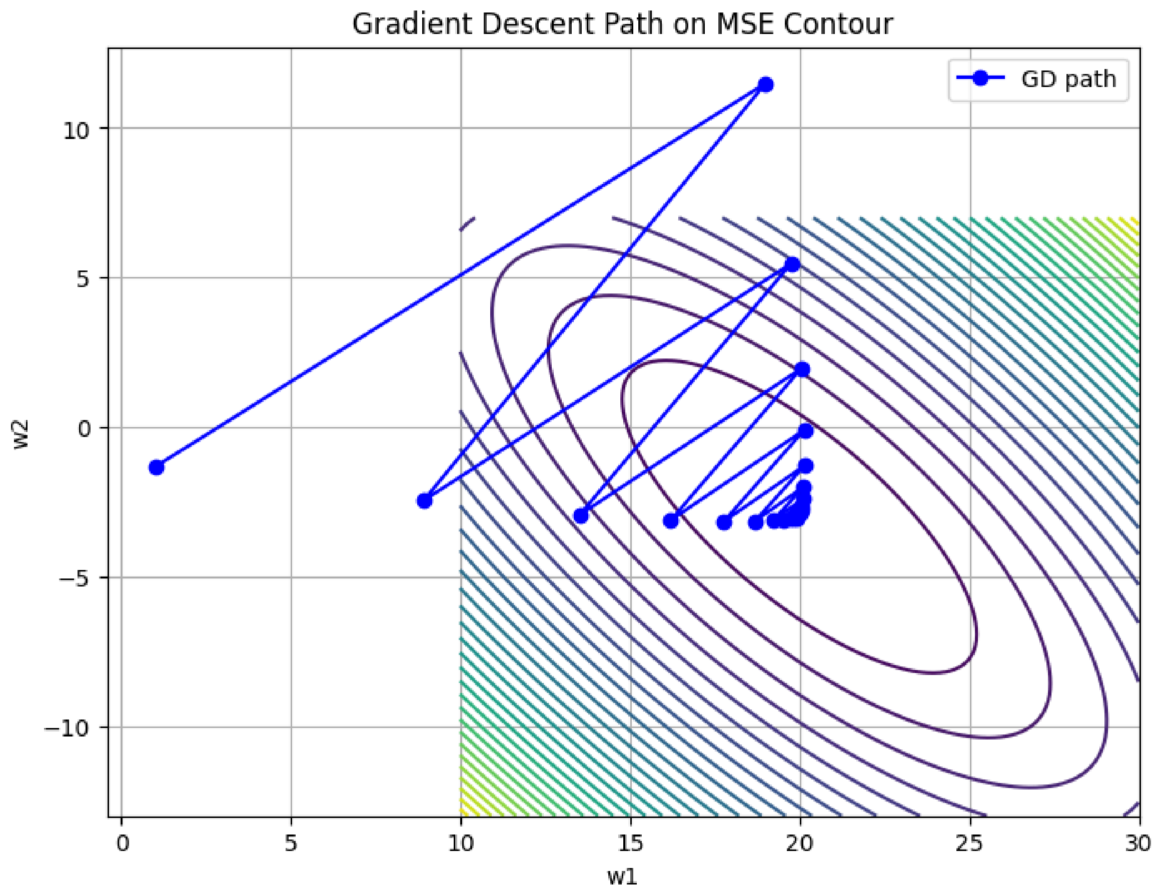
In [ ]:
```
def model(w, x):
    return np.dot(x, w)

# Define MSE loss function
def mse(w, model, X, Y):
    predictions = np.dot(X, w)
    return np.mean((Y - predictions)**2)

# Define gradient of MSE
def grad_mse(w, model, X, Y):
    N = len(Y)
    predictions = np.dot(X, w)
    error = predictions - Y
    grad = (2/N) * np.dot(X.T, error)
    return grad

in_dim = 2
out_dim = 1
limit = np.sqrt(6 / (in_dim + out_dim))
w0 = np.random.uniform(-limit, limit, size=(2,))
print("Initial weights (w0):", w0)

initial_loss = mse(w0, model, X, Y)
print("Initial MSE loss:", initial_loss)
```

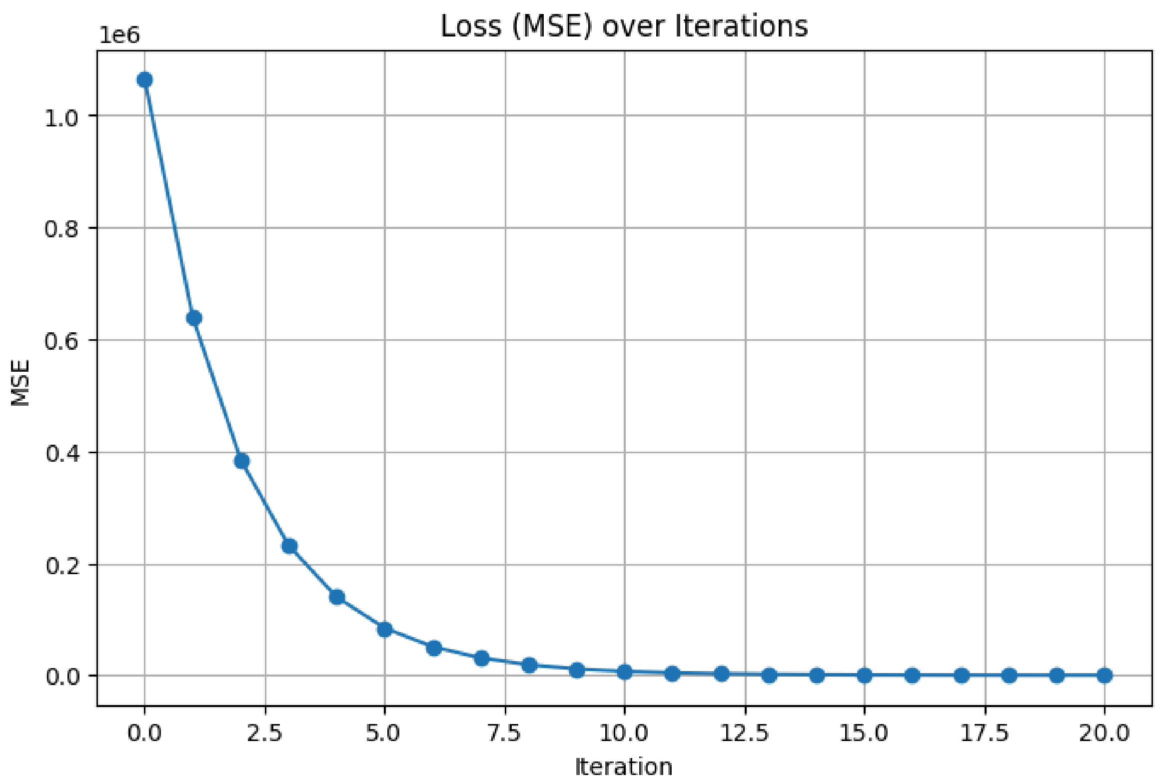
```
Initial weights (w0): [ 1.03260529 -1.32128993]
Initial MSE loss: 1064547.2959333684
```

We can then print the contour and how the vanilla gradient descent converges to our target point. I used the same parameters as the example.

I also plotted the total loss over our iterations to show that it decreases. We can also see that it converges to 0 just like the example.

In [ ]:
```
# Gradient Descent optimizer (batch)
def grad_desc_mse(K, w_init, learning_rate, loss_func, grad_func, verbose=True):
    w = w_init.copy()
    history = [loss_func(w, model, X, Y)]
    trajectory = [w.copy()]
    for _ in range(K):
        grad = grad_func(w, model, X, Y)
        w -= learning_rate * grad
        trajectory.append(w.copy())
        history.append(loss_func(w, model, X, Y))
    return np.array(trajectory), history

# Set hyperparameters
K = 20
learning_rate = 0.00015

# Run optimization
trajectory, history = grad_desc_mse(K, w0, learning_rate, mse, grad_mse)

# Contour plot of MSE landscape
w1_vals = np.linspace(10, 30, 100)
w2_vals = np.linspace(-13, 7, 100)
W1, W2 = np.meshgrid(w1_vals, w2_vals)
Z = np.array([[mse(np.array([w1, w2]), model, X, Y) for w1 in w1_vals] for w2 in

plt.figure(figsize=(8,6))
cp = plt.contour(W1, W2, Z, levels=30, cmap='viridis')
plt.plot(trajectory[:, 0], trajectory[:, 1], marker='o', color='blue', label='GD
plt.title('Gradient Descent Path on MSE Contour')
plt.xlabel('w1')
plt.ylabel('w2')
plt.legend()
plt.grid(True)
plt.show()

# Plot MSE loss over iterations
plt.figure(figsize=(8,5))
plt.plot(range(len(history)), history, marker='o')
plt.title('Loss (MSE) over Iterations')
plt.xlabel('Iteration')
plt.ylabel('MSE')
plt.grid(True)
plt.show()

# print convergence information
print("Final weights (w):", trajectory[-1])
print("Final MSE loss:", history[-1])
```






```
Final weights (w): [19.90656861 -3.02620454]
Final MSE loss: 144.64721257053787
```

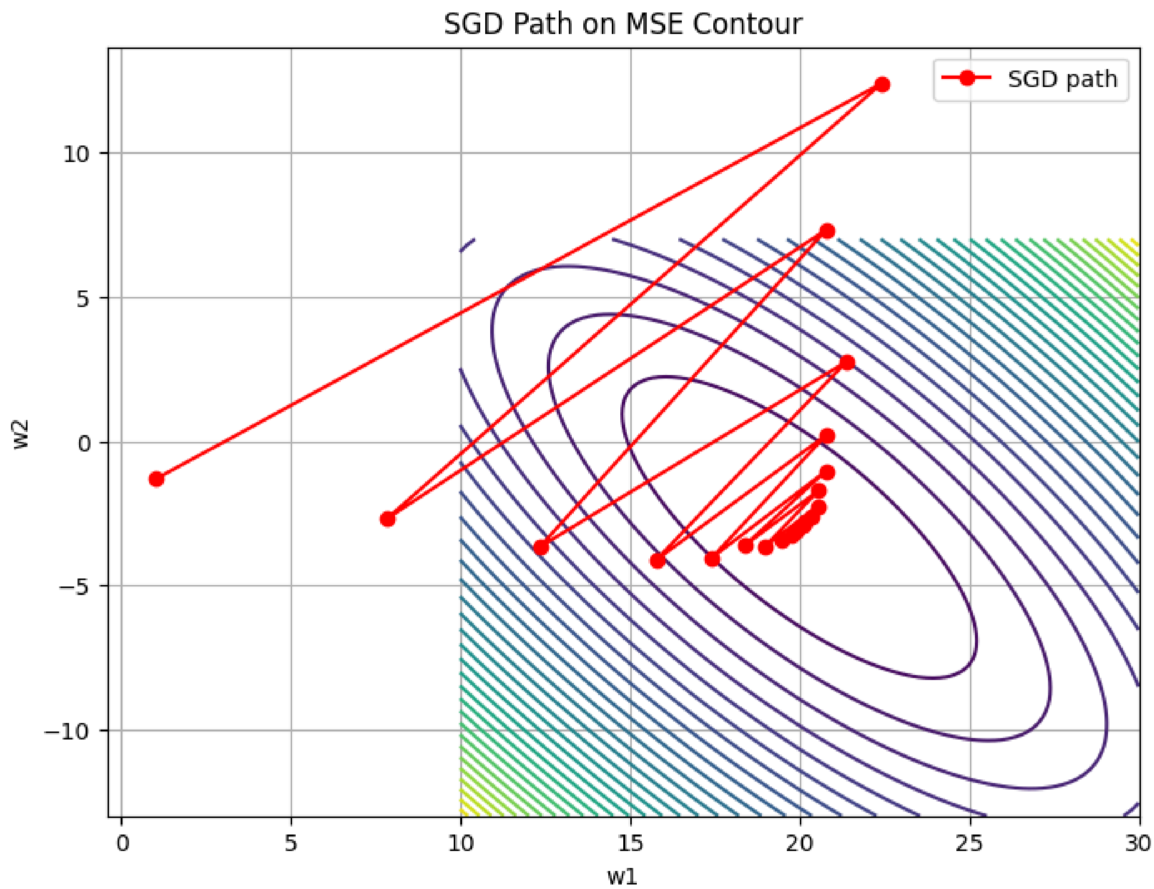
2. Stochastic gradient descent (SGD)

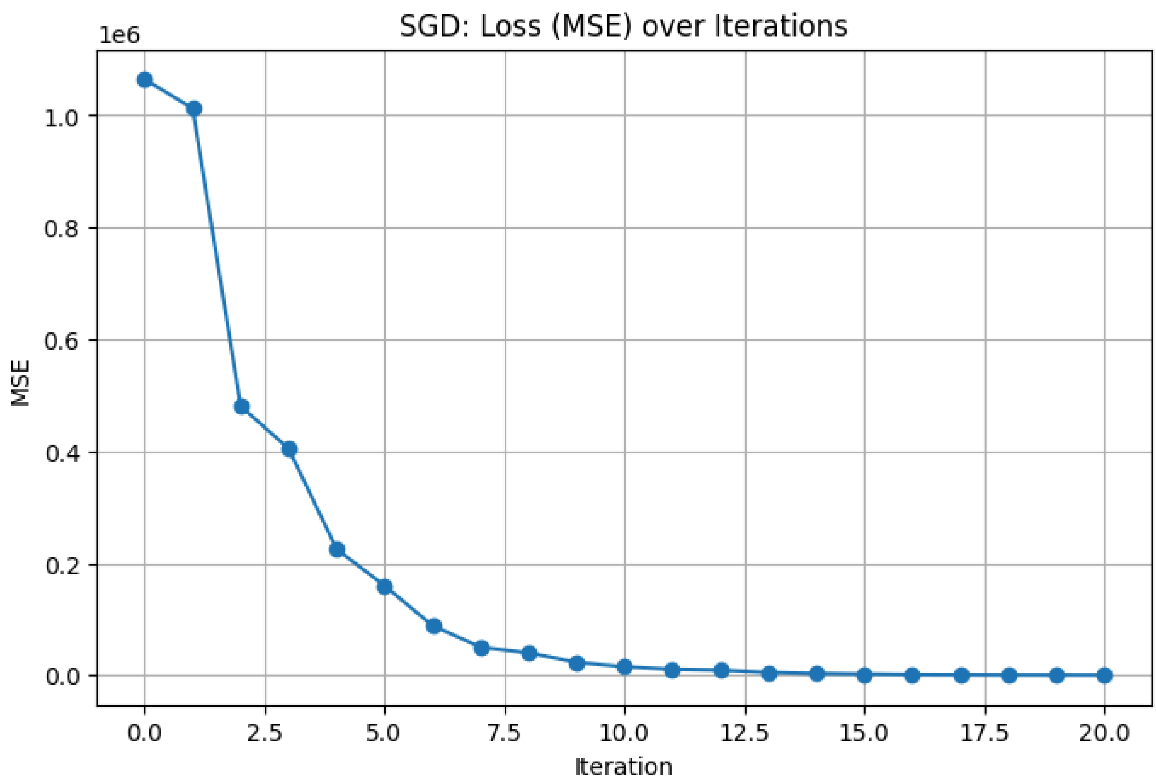
In [ ]:
```
def stochastic_grad_desc_mse(K, w_init, learning_rate, loss_func, grad_func, N,
    w = w_init.copy()
    history = [loss_func(w, model, X, Y)]
```

```
    trajectory = [w.copy()]
    batch_size = max(1, int(batch_fraction * N))

    for _ in range(K):
        rand_indices = np.random.choice(N, size=batch_size, replace=False)
        grad = grad_func(w, model, X[rand_indices], Y[rand_indices])
        old_w = w.copy()
        w -= learning_rate * grad
        trajectory.append(w.copy())
        history.append(loss_func(w, model, X, Y))

    return np.array(trajectory), history

def grad_mse_sampled(w, model, X_sample, Y_sample):
    N = len(Y_sample)
    predictions = np.dot(X_sample, w)
    error = predictions - Y_sample
    grad = (2/N) * np.dot(X_sample.T, error)
    return grad

K = 20
learning_rate = 0.00015

trajectory_sgd, history_sgd = stochastic_grad_desc_mse(K, w0, learning_rate, mse
```

In [ ]:

```
w1_vals = np.linspace(10, 30, 100)
w2_vals = np.linspace(-13, 7, 100)
W1, W2 = np.meshgrid(w1_vals, w2_vals)
Z = np.array([[mse(np.array([w1, w2]), model, X, Y) for w1 in w1_vals] for w2 in

plt.figure(figsize=(8,6))
cp = plt.contour(W1, W2, Z, levels=30, cmap='viridis')
plt.plot(trajectory_sgd[:, 0], trajectory_sgd[:, 1], marker='o', color='red', la
plt.title('SGD Path on MSE Contour')
plt.xlabel('w1')
plt.ylabel('w2')
plt.legend()
plt.grid(True)
plt.show()

plt.figure(figsize=(8,5))
plt.plot(range(len(history_sgd)), history_sgd, marker='o')
plt.title('SGD: Loss (MSE) over Iterations')
plt.xlabel('Iteration')
plt.ylabel('MSE')
plt.grid(True)
plt.show()
```





So as we can see, SGD is a bit less smooth when it comes to how the loss curve goes over the iterations.

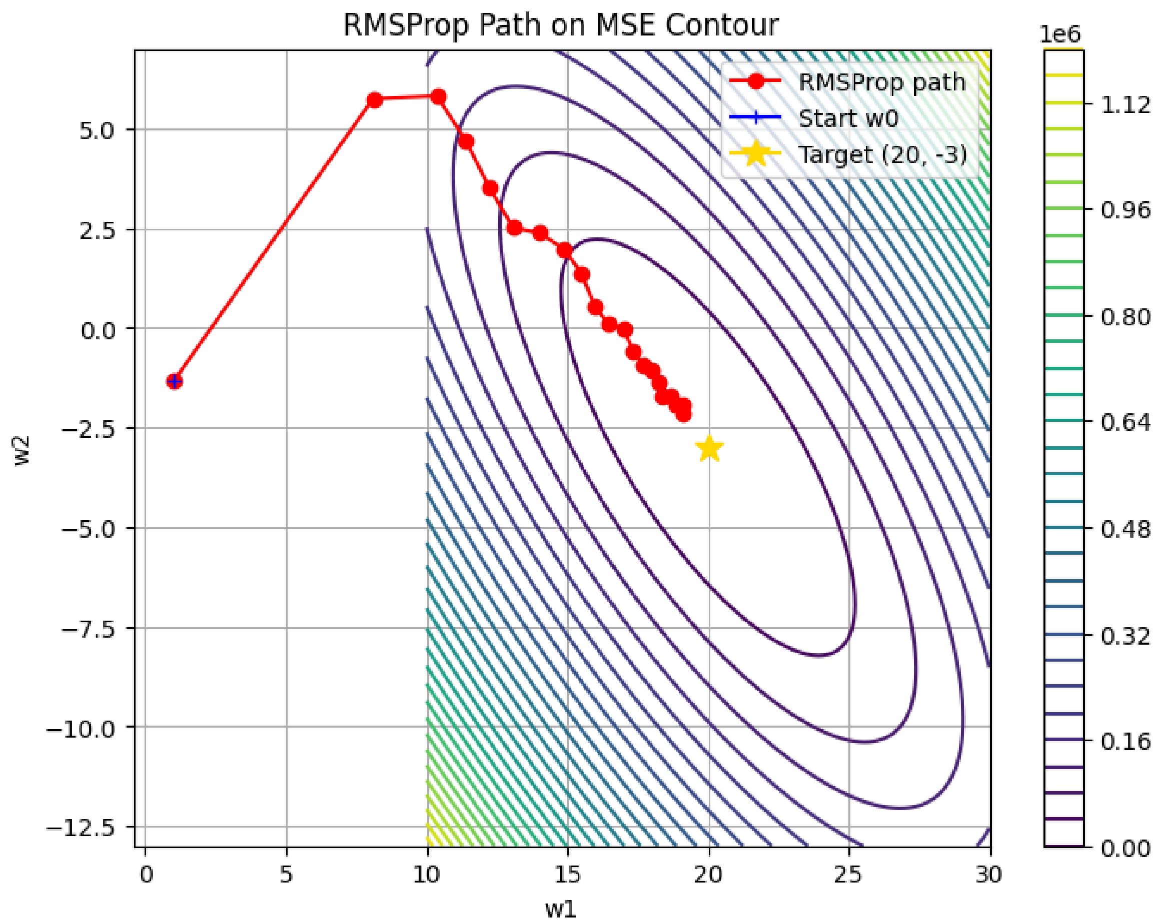
3. SGD with accumulated squared gradient: RMSProphe

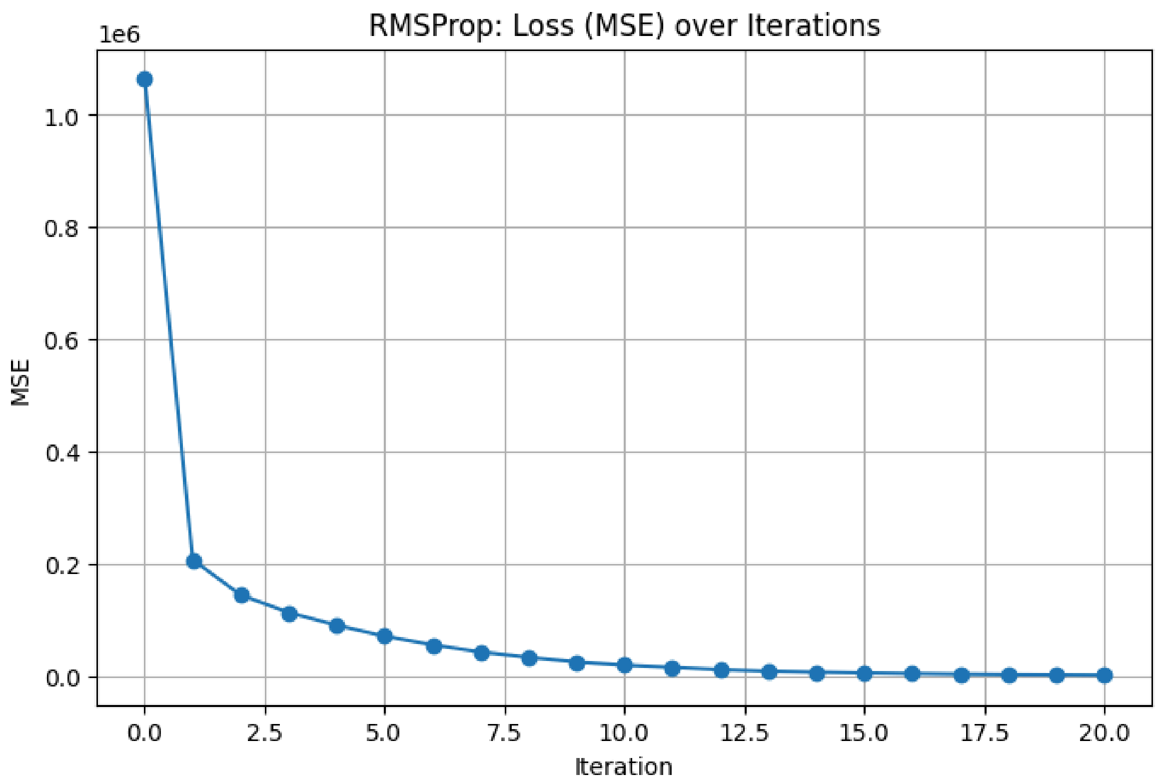
In [ ]:
```
def rmsprop_mse(K, w_init, learning_rate, loss_func, grad_func, N, rho=0.9, batc
    w = w_init.copy()
```

```python
    history = [loss_func(w, model, X, Y)]
    trajectory = [w.copy()]
    r = np.zeros_like(w)
    batch_size = max(1, int(batch_fraction * N))

    for _ in range(K):
        rand_indices = np.random.choice(N, size=batch_size, replace=False)
        grad = grad_func(w, model, X[rand_indices], Y[rand_indices])
        r = rho * r + (1 - rho) * grad**2
        old_w = w.copy()
        w -= (learning_rate / (np.sqrt(r) + delta)) * grad
        trajectory.append(w.copy())
        history.append(loss_func(w, model, X, Y))

    return np.array(trajectory), history

# Set hyperparameters
K = 20
learning_rate = 1.0
rho = 0.98

# Run RMSProp
trajectory_rms, history_rms = rmsprop_mse(K, w0, learning_rate, mse, grad_mse_sa
```

In [ ]:

```python
plt.figure(figsize=(8,6))
cp = plt.contour(W1, W2, Z, levels=30, cmap='viridis')
plt.colorbar(cp)
plt.plot(trajectory_rms[:, 0], trajectory_rms[:, 1], marker='o', color='red', la
plt.plot(w0[0], w0[1], marker='+', color='blue', label='Start w0')
plt.plot(20, -3, marker='*', color='gold', label='Target (20, -3)', markersize=1
plt.title('RMSProp Path on MSE Contour')
plt.xlabel('w1')
plt.ylabel('w2')
plt.legend()
plt.grid(True)
plt.show()

# %% [markdown]
# ### Plot the MSE loss over RMSProp iterations

# %%
plt.figure(figsize=(8,5))
plt.plot(range(len(history_rms)), history_rms, marker='o')
plt.title('RMSProp: Loss (MSE) over Iterations')
plt.xlabel('Iteration')
plt.ylabel('MSE')
plt.grid(True)
plt.show()
```



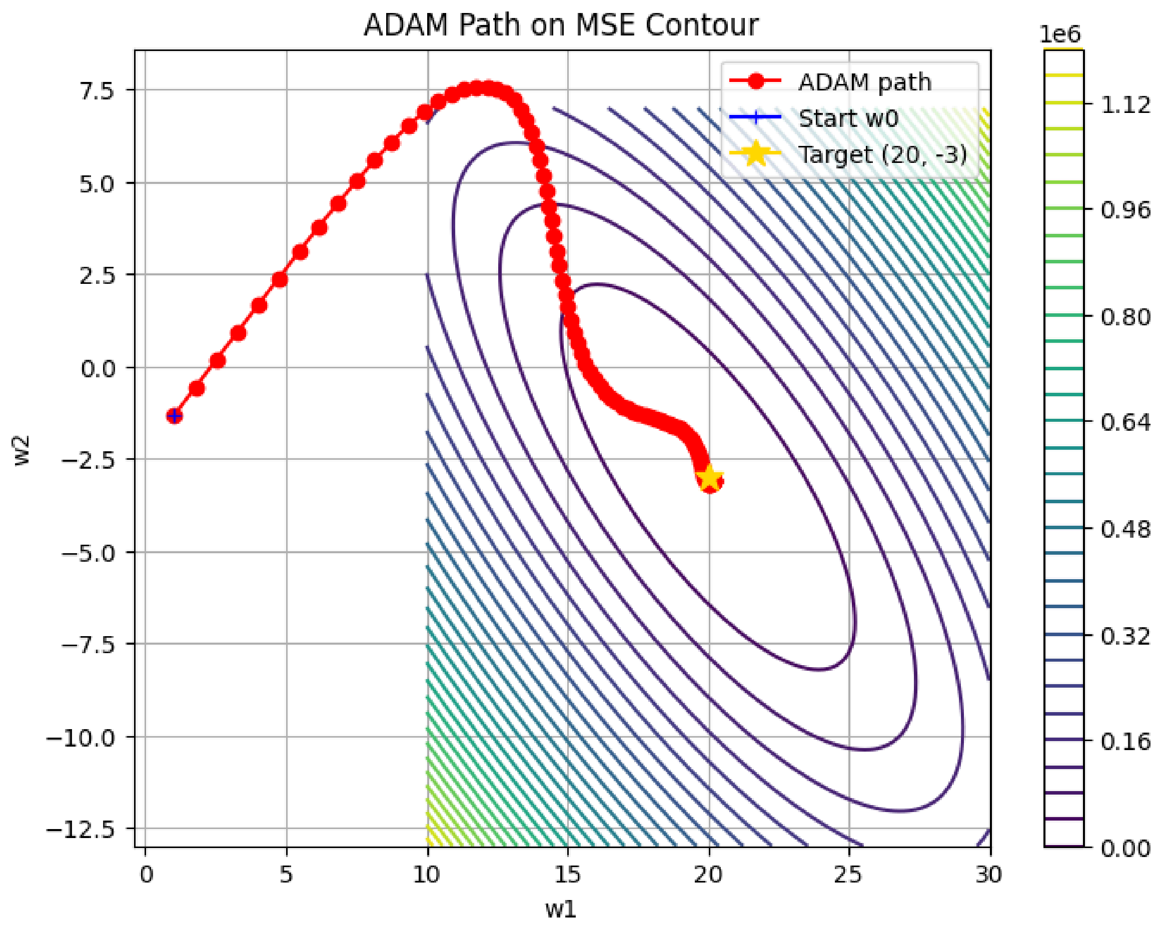


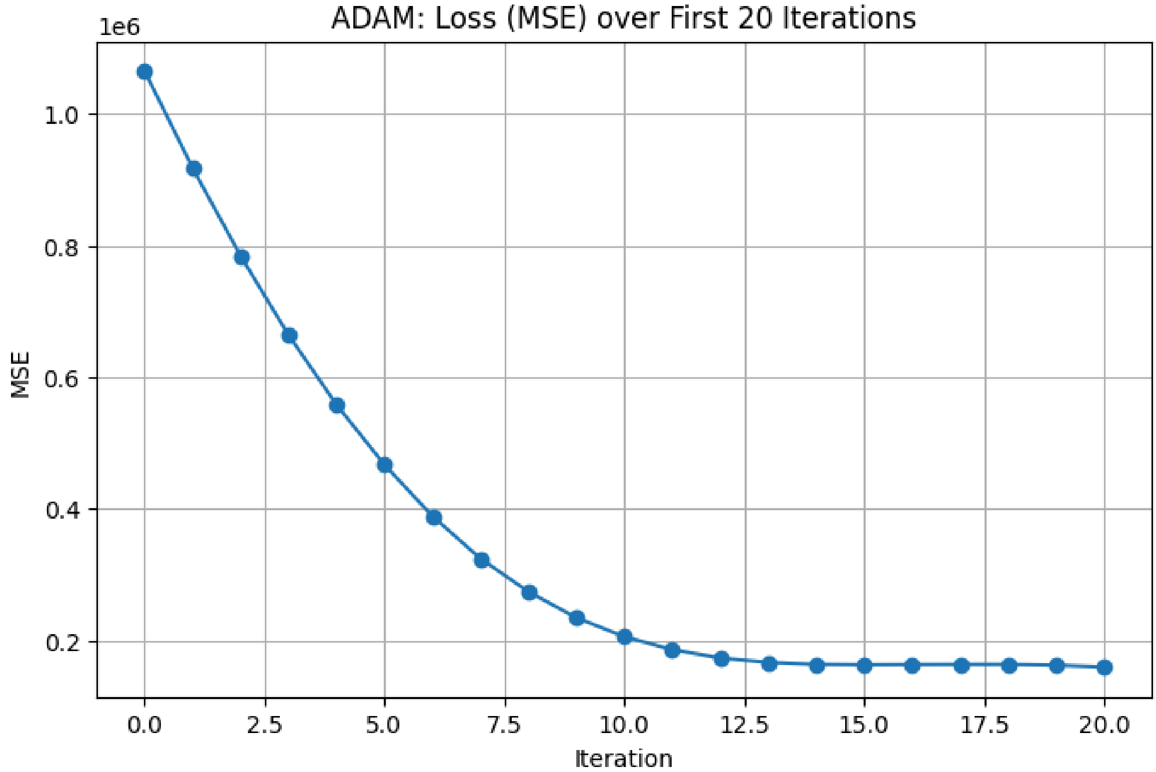
Because RMSprop has adaptive learning rate, we will see that the first couple of iiterations are very long steps and the algorithm kind of "locks in" on the target point. It handles early noisy updates well and doesent overshoot like the vanilla SGD sometimes does. This is a clear improvement over the vanilla SGD.

4. SGD with accumulated squared gradient: ADAM

In [ ]:
```
def adam_mse(K, w_init, learning_rate, loss_func, grad_func, N, rho1=0.9, rho2=0
    w = w_init.copy()
    history = [loss_func(w, model, X, Y)]
    trajectory = [w.copy()]
    s = np.zeros_like(w)  # First moment (momentum)
    r = np.zeros_like(w)  # Second moment (RMS)
    t = 0
    batch_size = max(1, int(batch_fraction * N))

    for _ in range(K):
        t += 1
        rand_indices = np.random.choice(N, size=batch_size, replace=False)
        grad = grad_func(w, model, X[rand_indices], Y[rand_indices])

        s = rho1 * s + (1 - rho1) * grad
        r = rho2 * r + (1 - rho2) * grad**2

        s_hat = s / (1 - rho1**t)
        r_hat = r / (1 - rho2**t)

        old_w = w.copy()
        w -= (learning_rate * s_hat) / (np.sqrt(r_hat) + delta)

        trajectory.append(w.copy())
        history.append(loss_func(w, model, X, Y))

    return np.array(trajectory), history

# Set hyperparameters (from the notebook's tuning)
K = 100
learning_rate = 0.75
rho1 = 0.9
rho2 = 0.999

# Run ADAM
trajectory_adam, history_adam = adam_mse(K, w0, learning_rate, mse, grad_mse_sam
```

In [ ]:
```
plt.figure(figsize=(8,6))
cp = plt.contour(W1, W2, Z, levels=30, cmap='viridis')
plt.colorbar(cp)
plt.plot(trajectory_adam[:, 0], trajectory_adam[:, 1], marker='o', color='red',
plt.plot(w0[0], w0[1], marker='+', color='blue', label='Start w0')
plt.plot(20, -3, marker='*', color='gold', label='Target (20, -3)', markersize=1
plt.title('ADAM Path on MSE Contour')
plt.xlabel('w1')
plt.ylabel('w2')
plt.legend()
plt.grid(True)
plt.show()

# Only show first 20 steps as in the MATLAB notebook
plt.figure(figsize=(8,5))
plt.plot(range(21), history_adam[:21], marker='o')
plt.title('ADAM: Loss (MSE) over First 20 Iterations')
plt.xlabel('Iteration')
plt.ylabel('MSE')
plt.grid(True)
plt.show()
```





As we can see, ADAM is much smoother in terms of stability because we can see that it is less sensitive to the initial learning rate.