Variants of stochastic gradient-based optimization

Steps

1. Setting the scene
2. Stochastic Gradient Descent (SGD) *(not implemented)*
3. SGD with adaptive learning rate *(implemented and optimized using grid search)*
4. SGD with adaptive learning rate *(implemented and optimized using random search)*

Setting the scene

During learning, we optimize the mean squared error MSE of the models m for the model parameters $\mathbf{w}$:

$$MSE(\mathbf{w}, m, X, Y) = \frac{1}{N}\sum_{i=1}^{N}(y_i - m(\mathbf{w}, \mathbf{x}_i))^2$$

In other words, we find $\arg\min_{\mathbf{w}} MSE(\mathbf{w}, m, X, Y)$.

We will reuse some functions defined in the notebook "Learn an XOR Neural Network using gradient-based optimization" including:

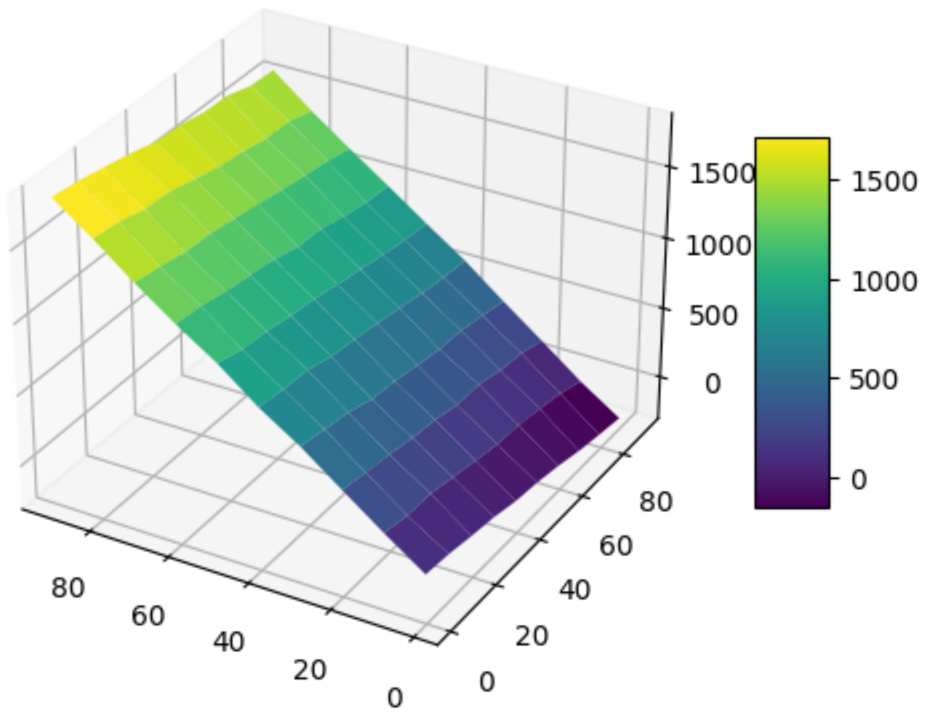
1. The mean squared error function `mse` (loss function).
2. The gradient of the mean squared error function `grad_mse` (gradient of the loss function).
3. The gradient descent function for the loss function `grad_desc_mse` .
4. The 3D surcace and contour plot function `plot3D` .

In [ ]:
```
import numpy as np
import matplotlib.pyplot as plt

def mse(ws, m, X, Y):
    N = len(X)
    err = 0
    for i in range(N):
        y_hat = m(ws, X[i])
        err += (Y[i] - y_hat)**2
    return err / N

def grad_mse(ws, m, grads, X, Y):
    N = len(X)
    M = len(ws)
    grad_ws = np.zeros((M))
    for i in range(N):
        xi = X[i,:]
        yi = Y[i]
        tmp = yi - m(ws, xi)
        for j in range(M):
            grad_ws[j] = grad_ws[j] + tmp*grads[j](ws, xi)
    grad_ws = grad_ws / -2
    return grad_ws

def grad_desc_mse(K, ws, learning_eps, loss, grad_loss, verbose):
    hist = np.zeros((K+1))
    hist[0] = loss(ws)
    for k in range(K):
        grad_ws = grad_loss(ws)
        old_ws = ws
        ws = old_ws - learning_eps * grad_ws
        if verbose:
            plt.plot([old_ws[0], ws[0]], [old_ws[1], ws[1]])

        hist[k+1] = loss(ws)
    return ws, hist

def plot3d(f,A,B,real3d):
    vectorized_func = np.vectorize(f)
    Z = vectorized_func(A,B)
    if real3d:
        fig = plt.figure()
        ax = fig.add_subplot(111, projection='3d')
        surf = ax.plot_surface(A, B, Z, cmap='viridis')
        fig.colorbar(surf, shrink=0.5, aspect=5)
        ax.invert_xaxis()
    else:
        fig = plt.figure()
        ax = fig.add_subplot(111)
        surf = ax.contour(A, B, Z, cmap='viridis')
        fig.colorbar(surf, shrink=0.5, aspect=5)
    return fig, ax
```

First we generate sample data points. The generator function is $y = 20x_1 - 3x_2$. We sample data at integer points $x_{i,1} \times x_{i,2} \in [1 \dots N] \times [1 \dots N], N = 100$ and add a random error to y_i that is normally distributed proportional to $\mathcal{N}(0, 10)$.

Below we plot the function.

In [ ]:
```
N = 100
XX = np.array(np.meshgrid(np.arange(1,N+1), np.arange(1,N+1))).T.reshape(-1, 2)
a10 = 20
a20 = -3

X1 = XX[:,0]
X2 = XX[:,1]

f0 = lambda x1, x2: a10*x1 + a20*x2
f = lambda x1,x2,r: a10*x1 + a20*x2 + r

np.random.seed(42)
R = np.transpose(np.random.normal(0, 10, len(XX)))
Y = np.vectorize(f)(X1,X2,R)
A,B = np.meshgrid(np.arange(1, N+1, N/10), np.arange(1, N+1, N/10))
ff = lambda x1,x2: f(x1,x2,np.random.normal(0, 10))

plot3d(ff, A,B, True)
plt.show()
```



The model that we use throughout this notebook is a simple linear Neural Network model. It consists of one neuron connected to the input $\mathbf{x}$ and an identity, i.e., no effective, activation function. The neuron and the whole model m_1 implements $m_1(\mathbf{w}, \mathbf{x}) = \mathbf{w}^T\mathbf{x}$.

In [ ]:
```
m1 = lambda ws,x: ws[0] * x[0] + ws[1] * x[1]
mse1 = lambda ws: mse(ws, m1, XX, Y)
```

As the Tensorflow default, we implement the Glorot uniform initializer for setting the initial weights $\mathbf{w}_0$. It draws samples from a uniform random distribution within $[-limit, limit]$, where $limit = \sqrt{\frac{6}{in+out}}$, and where in and out is the number of input and output units, resp.

In [ ]:
```
import math
import random

random.seed(42)
input = 2
out = 2
limit = math.sqrt(6 / (input + out))
ws0 = [random.uniform(-limit, limit), random.uniform(-limit, limit)]
print(ws0)
```

```
[0.3415245126916837, -1.1634812830144055]
```

We assess the loss MSE of m_1 for this initial weights setting.

In [ ]:
```
mse1(ws0)
```

Out[ ]:
```
1134789.243254444
```

The gradient of $MSE(\mathbf{w})$ for any $\mathbf{w}$ is defiend as:

$$\begin{aligned}
\nabla_{MSE}(\mathbf{w}) &= \left[\frac{\partial MSE(\mathbf{w})}{\partial w_1}, \frac{\partial MSE(\mathbf{w})}{\partial w_2}\right]^T \\
&= \frac{1}{N}\left[\frac{\partial \sum_{i=1}^N (y_i - m_1(\mathbf{w}, \mathbf{x}_i)^2}{\partial w_1}, \frac{\partial \sum_{i=1}^N (y_i - m_1(\mathbf{w}, \mathbf{x}_i))^2}{\partial w_2}\right]^T \\
&= \frac{1}{N}\left[\sum_{i=1}^N 2(y_i - m_1(\mathbf{w}, \mathbf{x}_i))\frac{-\partial m_1(\mathbf{w}, \mathbf{x}_i)}{\partial w_1}, \sum_{i=1}^N 2(y_i - m_1(\mathbf{w}, \mathbf{x}_i))\frac{-\partial m_1(\mathbf{w}, \mathbf{x}}{\partial w_2}\right. \\
&= -\frac{2}{N}\left[\sum_{i=1}^N (y_i - m_1(\mathbf{w}, \mathbf{x}_i))\frac{\partial m_1(\mathbf{w}, \mathbf{x}_i)}{\partial w_1}, \sum_{i=1}^N (y_i - m_1(\mathbf{w}, \mathbf{x}_i))\frac{\partial m_1(\mathbf{w}, \mathbf{x}_i)}{\partial w_2}\right]^T
\end{aligned}$$

We can plug in the function m_1 and the first derivative of m_1 wrt. w_1 and w_2 resp.

$$\begin{aligned}
\frac{\partial m_1(\mathbf{w}, \mathbf{x}_i)}{\partial w_1} &= \frac{\partial \mathbf{w}^T \mathbf{x}_i}{\partial w_1} = \frac{\partial w_1 x_{i,1} + w_2 x_{i,2}}{\partial w_1} = x_{i,1} \\
\frac{\partial m_1(\mathbf{w}, \mathbf{x}_i)}{\partial w_2} &= \frac{\partial \mathbf{w}^T \mathbf{x}_i}{\partial w_2} = \frac{\partial w_1 x_{i,1} + w_2 x_{i,2}}{\partial w_2} = x_{i,2}
\end{aligned}$$

We have already defined the function m_1. Let's also define the functions of the first derivative of m_1 wrt. w_1 and w_2 resp. For the sake of generality, we keep $\mathbf{w}$ as a formal parameter `ws` even though it is actually not needed for derivatives of this concrete model m_1.

In [ ]:
```
grad1 = lambda ws, x: x[0]
grad2 = lambda ws, x: x[1]
gradients1 = [grad1, grad2]
```

The gradient $\nabla_{MSE}(\mathbf{w})$ has been defined using m_1 and the first derivative of m_1 wrt. w_1 and w_2, resp., as parameters.

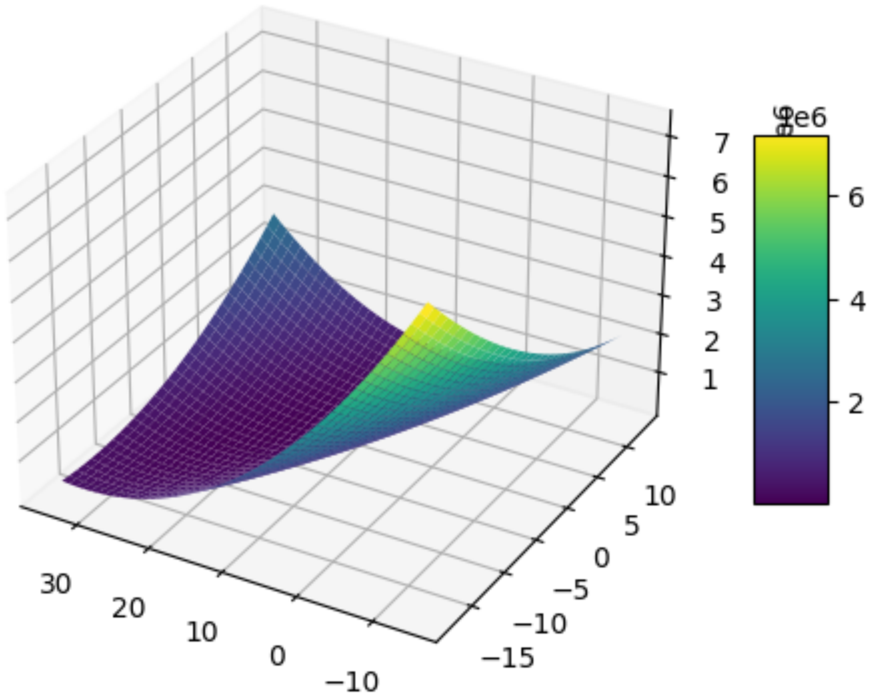
The gradient descent function optimizes $\mathbf{w}$ by iterating over:

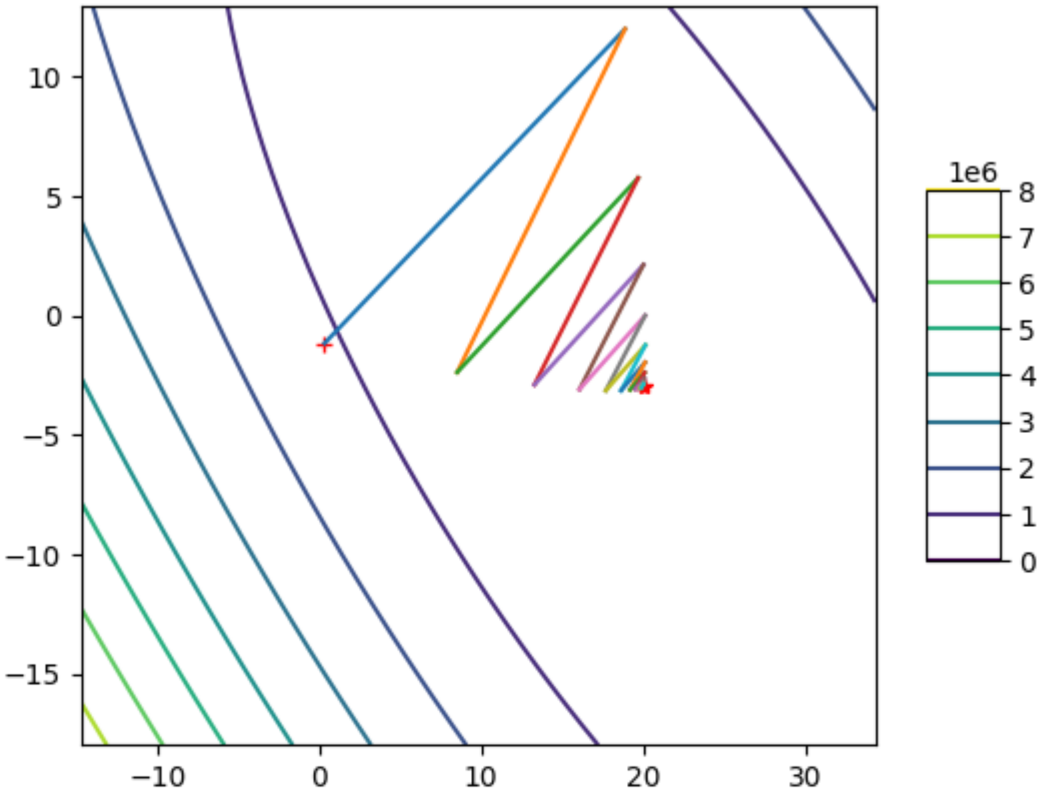
$$\mathbf{w}_{k+1} = \mathbf{w}_k - \varepsilon \nabla_{MSE}(\mathbf{w}_k)$$

staring with $\mathbf{w}_0$.

Below we apply the gradient descent function minimizing MSE for the model m_1. We plot the MSE for each step k in the iteration as a function of the current parameter setting $\mathbf{w}_k$. We also marked the starting point $\mathbf{w}_0$ with a `+` and the (ideal) minimum $(20, -3)$ with a `*`.

In [ ]:
```
f = lambda a,b : mse1([a,b])

A,B = np.meshgrid(np.arange(min(a10, ws0[0])-15, max(a10,ws0[0])+15), np.arange(min
plot3d(f,A,B, True)
plt.show()

plot3d(f, A, B, False)

plt.plot(a10, a20,'*r')
plt.plot(ws0[0], ws0[1],'+r')

#gradient descent
grad_loss = lambda ws: grad_mse(ws, m1, gradients1, XX, Y)
K = 20
learning_eps = 0.00000006 # needed to change the learning rate. Otherwise I got the
[ws, history] = grad_desc_mse(K, ws0, learning_eps, mse1, grad_loss, True)
```





Original approach with two hyper-parameters using an orginary grid search

SGD with adaptive learning rate

```
In [ ]: # SGD
        grad_loss2 = lambda ws, randinces: grad_mse(ws, m1, gradients1, XX[randinces, :], Y
```

The learning rate ε is adapted in each iteration, e.g., exponentially by $\varepsilon_{k+1} = (1-\alpha)\varepsilon_k$ with α a new hyper-parameter.

```
In [ ]: def stochastic_adaptive_grad_desc_mse(K, ws, learning_eps, loss, grad_loss, N, alph
            batch_size = int(N*0.01)
            hist = np.zeros((K+1))
            hist[0] = loss(ws)
            for k in range(K):
                randices = np.random.choice(np.arange(0, N), size=batch_size, replace=False
                grad_ws = grad_loss(ws, randices)
                old_ws = ws
                ws = old_ws - learning_eps * grad_ws
                learning_eps = (1-alpha) * learning_eps
                if verbose:
                    plt.plot([old_ws[0], ws[0]], [old_ws[1], ws[1]])
                hist[k+1] = loss(ws)
            return ws, hist
```

Now I need to define a grid based approach to search for the optimal hyper-parameters. When tuning the hyper-parameter for a model I should consider cross validation. However, I assume that this excercise is about the advantages and disadvantages of the optimization strategies. Therefore, I neglected cross validataion and performed an ordinary grid search.

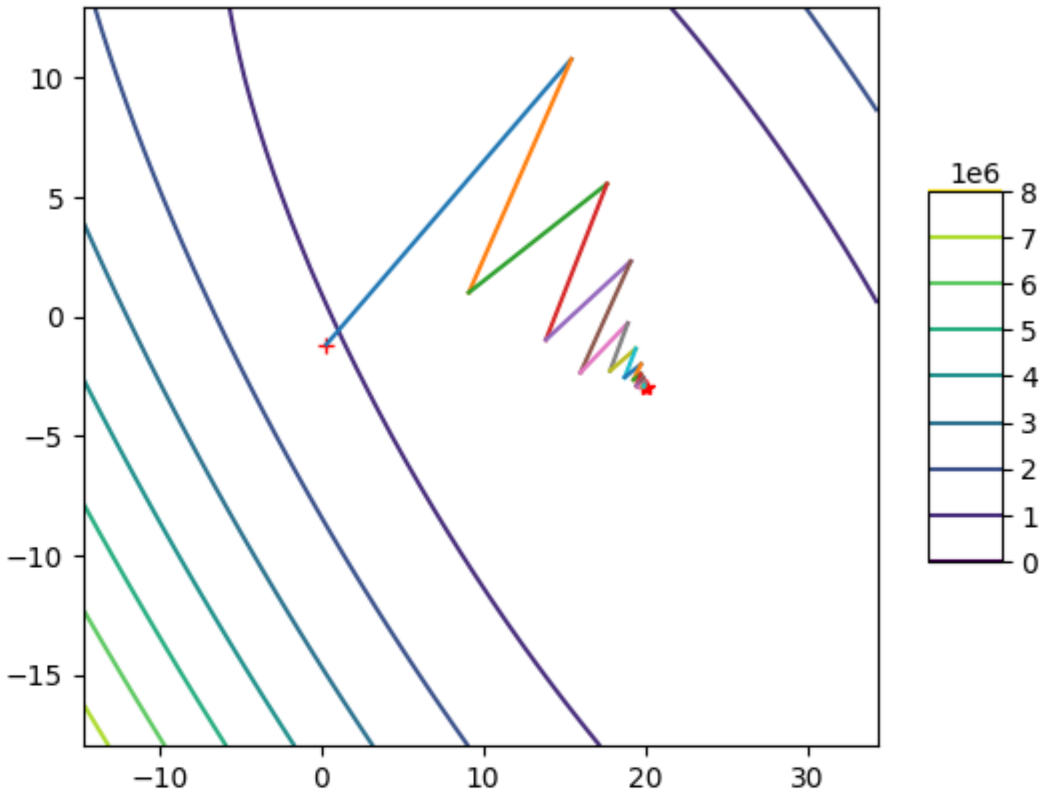
```
In [ ]: param_grid = {
            'learning_eps': [6e-5, 3e-5, 1e-5, 8e-6, 7e-6, 6e-6, 5e-6, 3e-6, 1e-6, 8e-7, 6e
            'alpha': [1e-5,3e-5,1e-4,3e-4,1e-3,3e-3,1e-2,3e-2]
        }

        best_score = 10000000
        best_params = None

        for learning_eps in param_grid['learning_eps']:
            for alpha in param_grid['alpha']:
                np.random.seed(42) # to be fair with the selection of mini batches in the w
                [ws, history] = stochastic_adaptive_grad_desc_mse(K, ws0, learning_eps, mse

                score = mse1(ws)
                if score < best_score:
                    best_score = score
                    best_params = {'learning_eps': learning_eps, 'alpha': alpha}

        print(best_params)
        print(best_score)

        {'learning_eps': 6e-06, 'alpha': 1e-05}
        109.2116509274781
```

Here, the optimal hyper-parameter according to my search are:

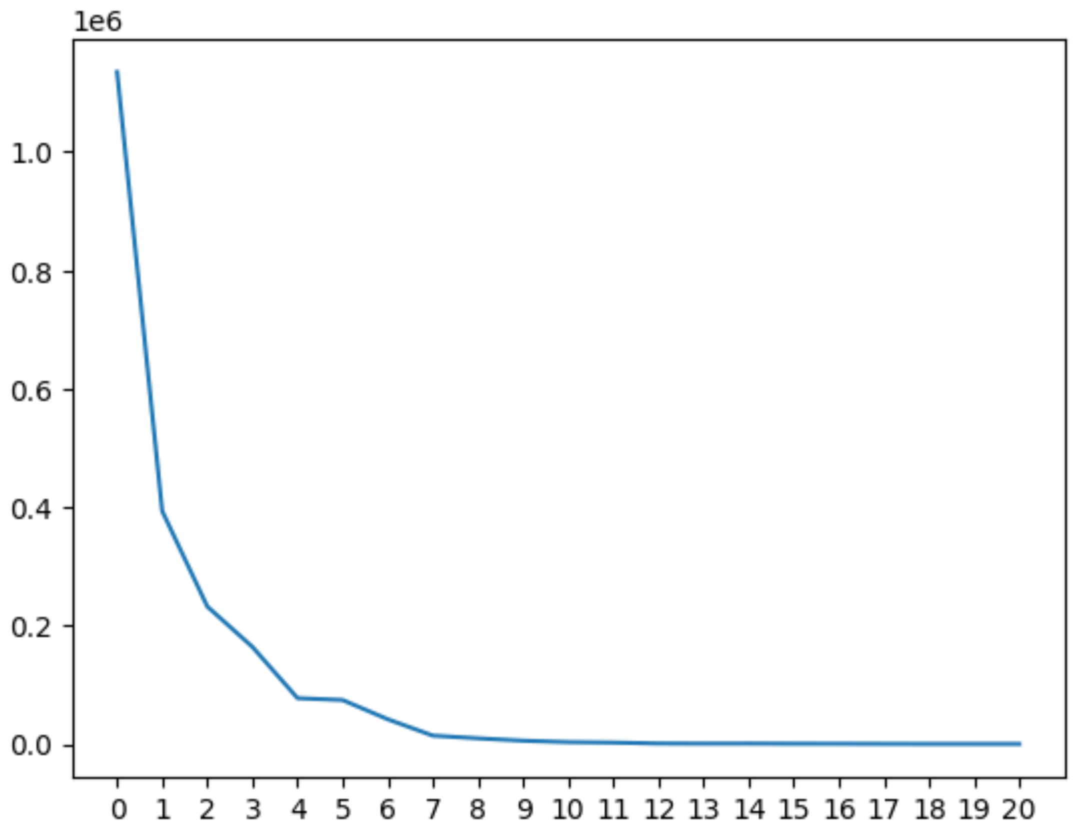
- $\varepsilon = 6e - 6$
- $\alpha = 0.00001$

Now I plugged it into the algorithm again and plotted the history of the search and the learning rate.

In [ ]:
```
plot3d(f, A, B, False)
plt.plot(a10, a20,'*r')
plt.plot(ws0[0], ws0[1],'+r')

[ws, history1] = stochastic_adaptive_grad_desc_mse(K, ws0, best_params['learning_ep
```



In [ ]:
```
plt.plot(range(len(history1)), history1)
plt.xticks(range(len(history1)))
plt.show()
```



Now with advanced optimization approach

I decided to choose random search performed with 1000 iterations. The scope of parameters was not changed.

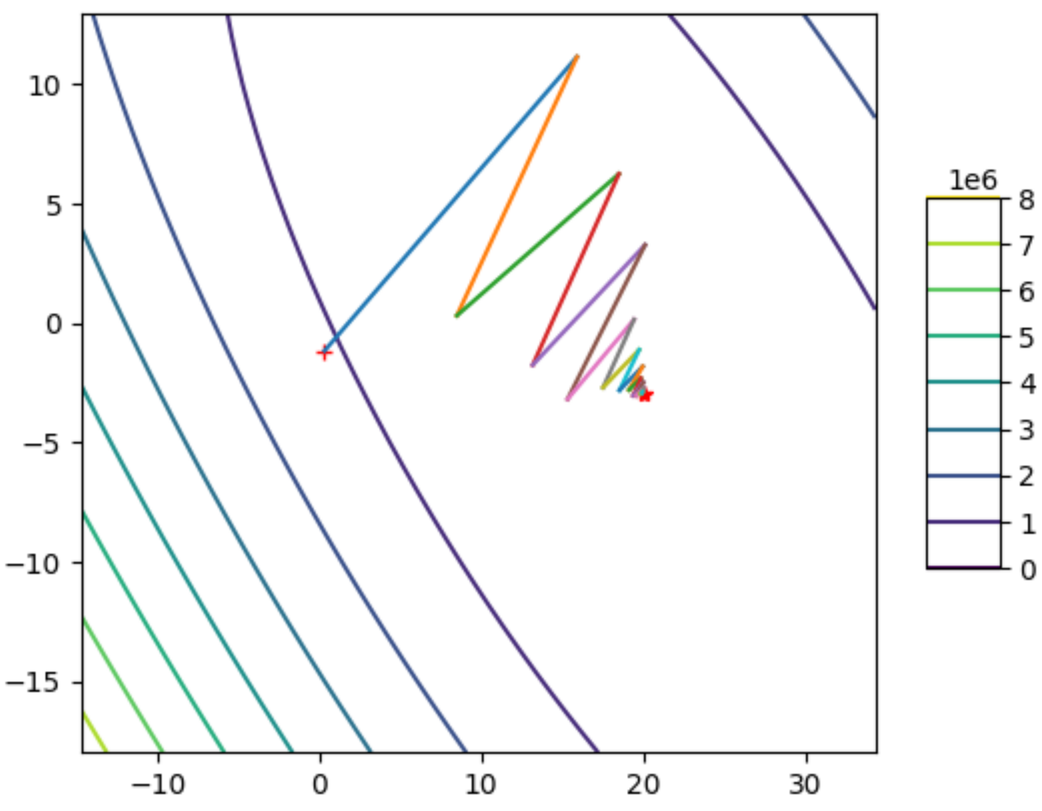
In [ ]:
```
from scipy.stats import uniform
from tqdm import tqdm

def sample_params(param_dist, random_state):
    params = {}
    for key, dist in param_dist.items():
        params[key] = dist.rvs(random_state = random_state)
    return params

param_dist = {
    'learning_eps': uniform(6e-7,6e-5),
    'alpha': uniform(1e-5,3e-2)
}

n_iter = 1000
best_score = 10000000
best_params = None

for i in tqdm(range(n_iter)):
    params = sample_params(param_dist, i)
    learning_eps = params['learning_eps']
    alpha = params['alpha']
    np.random.seed(42) # to be fair with the selection of mini batches in the whole
    [ws, history] = stochastic_adaptive_grad_desc_mse(K, ws0, learning_eps, mse1, g

    score = mse1(ws)
    if score < best_score:
        best_score = score
        best_params = {'learning_eps': learning_eps, 'alpha': alpha}

print(best_params)
print(best_score)
```

```
100%|██████████| 1000/1000 [01:54<00:00,  8.76it/s]
{'learning_eps': 6.18649720031148e-06, 'alpha': 0.0028032486001557397}
110.2136741319373
```

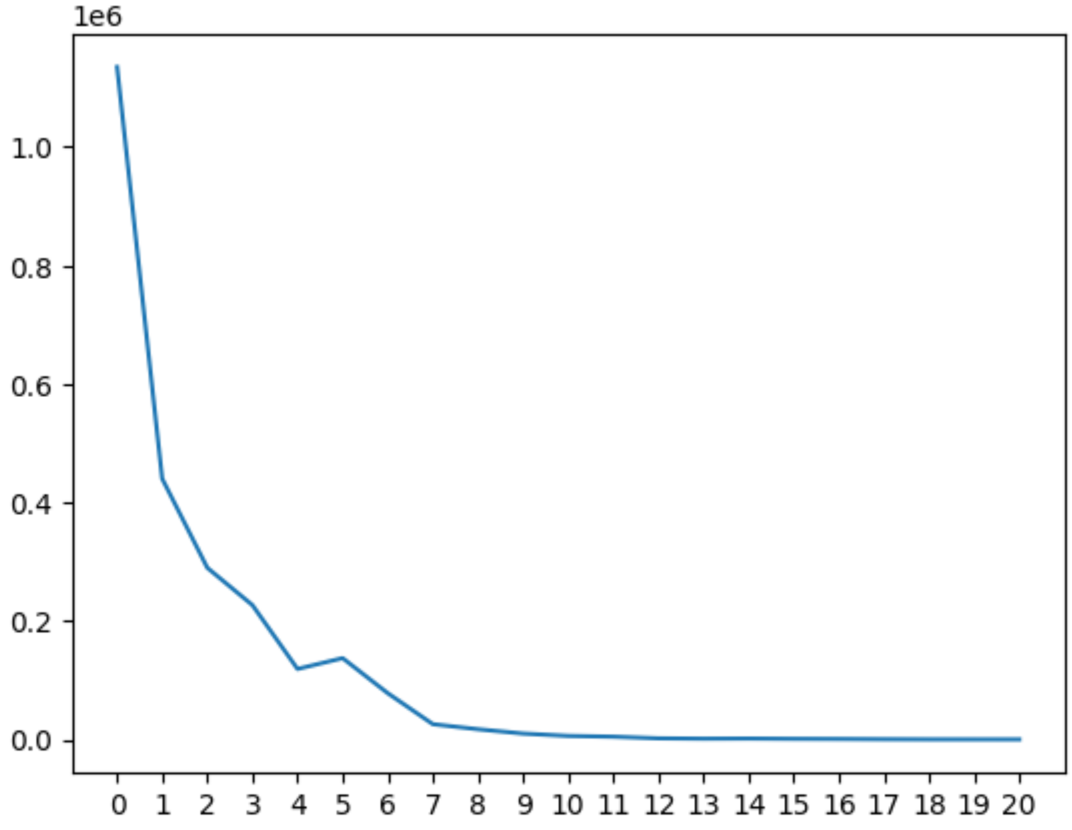
Here, the optimal hyper-parameter according to my random search are:

- $\varepsilon = 6.18649720031148e - 6$
- $\alpha = 0.0028032486001557397$

In [ ]:
```
plot3d(f, A, B, False)
plt.plot(a10, a20,'*r')
plt.plot(ws0[0], ws0[1],'+r')

[ws, history2] = stochastic_adaptive_grad_desc_mse(K, ws0, best_params['learning_ep
```



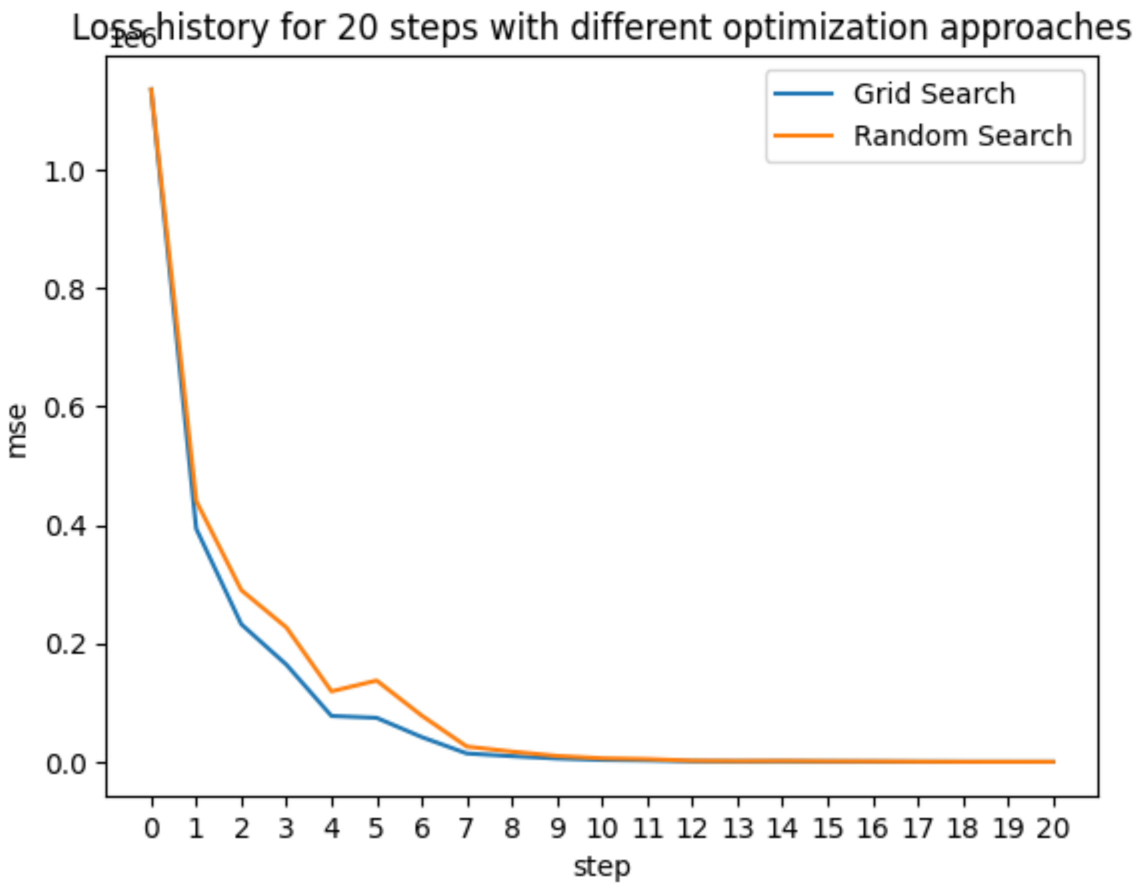
In [ ]:
```
plt.plot(range(len(history2)), history2)
plt.xticks(range(len(history2)))
plt.show()
```



Comparison

Here I plotted the learning rates of the two approaches choosen in one diagram

```
In [ ]: plt.plot(range(len(history1)), history1, label='Grid Search')
        plt.plot(range(len(history2)), history2, label='Random Search')
        plt.title('Loss history for 20 steps with different optimization approaches')
        plt.legend()
        plt.ylabel('mse')
        plt.xlabel('step')
        plt.xticks(range(len(history2)))
        plt.show()
```



Interpretation

One can see, that the trajectory of the loss curve is more direct/steeper with the parameters found in grid search approach. Especially in step 1 to 8, the gradient decent with parameters found in random search made wider steps. Hence, the flatter trajectory of the loss curve.

Additionally, the random search did not find a set of parameters coming with a lower loss than with the grid search approach, i.e. random search: 110.21, and grid search: 109.21. However, the random search ran for 1000 iterations and took, therefore, longer than the grid search, where 88 iterations were needed.

So, in the end, it might be more reasonable to test specific parameter settings in a grid, when having just a few parameters. In cases, when there are more parameters, it might be helpful to ran a random search to get an idea of suitable settings of the parameters and, thus, narrow down the value space for each of them. After that, a grid search might lead to better insights about parameter values, since one knows the tested parameters, which is not the case in random search (unless you log them). Also if one has no clue about a reasonable value of a hyper-parameter, random search and other advanced techniques could help to narrow down the reasonable value scope for several parameters, before setting up intended values in a grid search.