# Variants of stochastic gradient-based optimization

## Steps

1. Setting the scene
2. Stochastic Gradient Descent (SGD) *(implemented)*
3. SGD with adaptive learning rate *(implemented and optimized using grid search)*
4. SGD with momentum *(implemented and optimized using grid search)*
5. SGD with accumulated squared gradient: AdaGrad *(not implemented)*
6. SGD with accumulated squared gradient: RMSProp *(not implemented)*
7. SGD with accumulated squared gradient: ADAM *(not implemented)*

## 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:

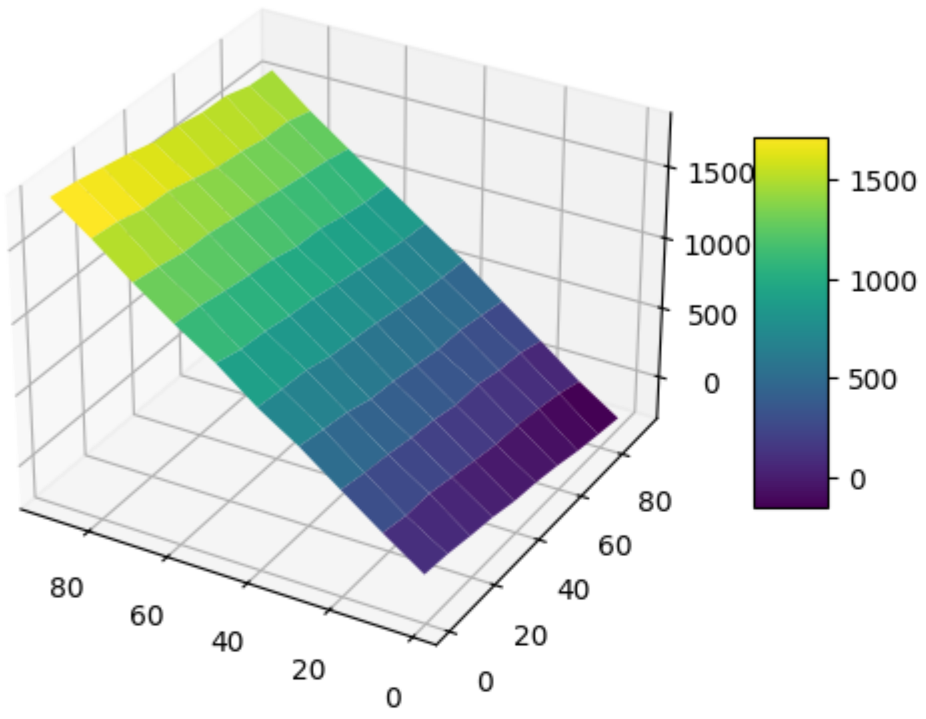
1. The mean squared error function `mse` (loss function).
2. The gradient of the mean squared error function `grad_mse` (gradient of the loss function).
3. The gradient descent function for the loss function `grad_desc_mse` .
4. The 3D surcace and contour plot function `plot3D` .

In [ ]:
```python
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 [ ]:
```python
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:

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

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.

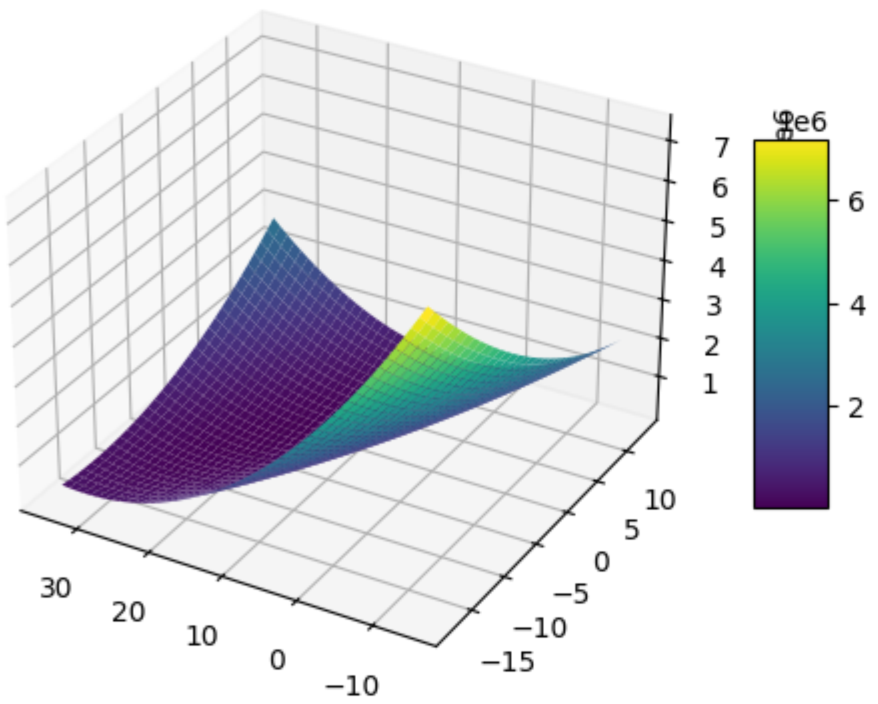
The gradient descent function optimizes $\mathbf{w}$ by iterating over:

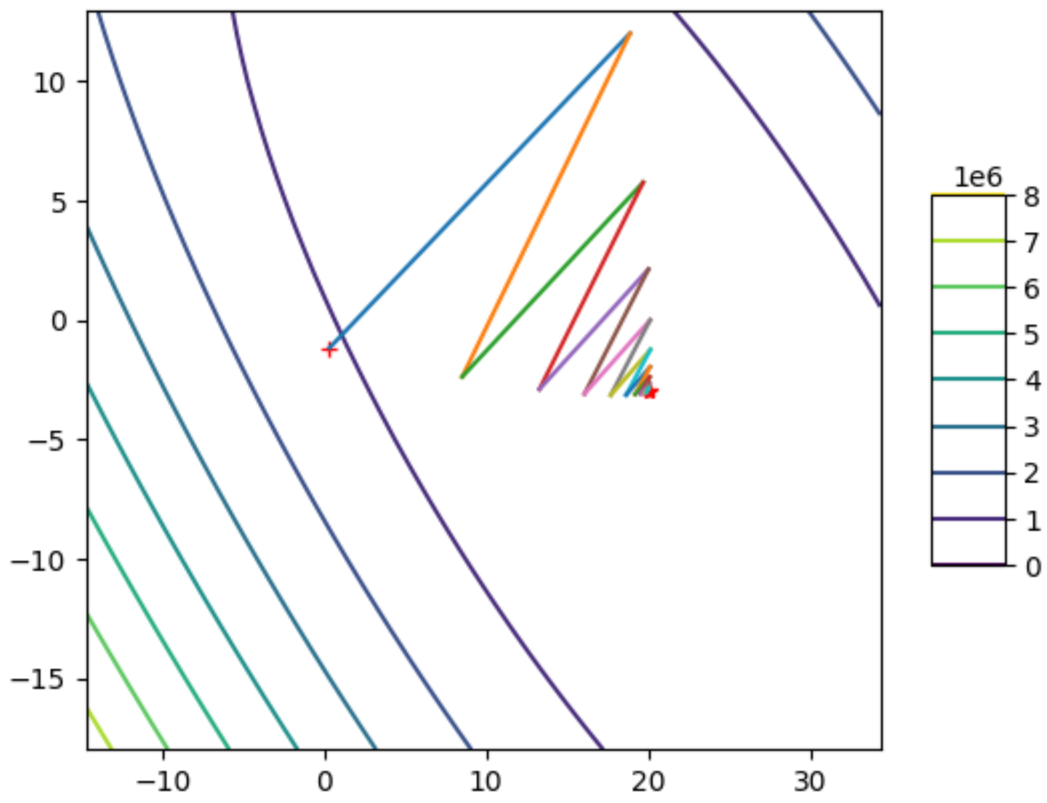
$$\mathbf{w}_{k+1} = \mathbf{w}_k - \varepsilon \nabla_{MSE}(\mathbf{w}_k)$$

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 `*`.

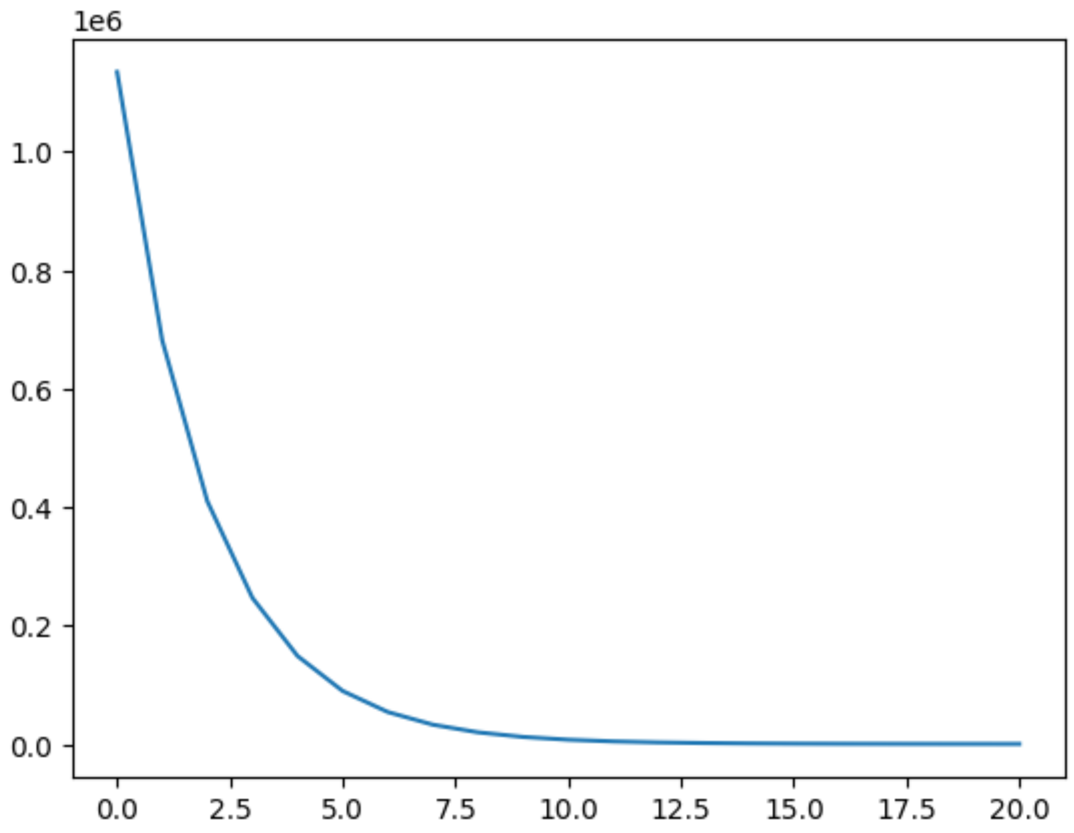
In [ ]:
```
f = lambda a,b : mse1([a,b])

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)
```





*The history plot shows the convergence of the algorithm. After ca. $k = 11$ iterations, the loss $MSE$ is almost zero.*

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



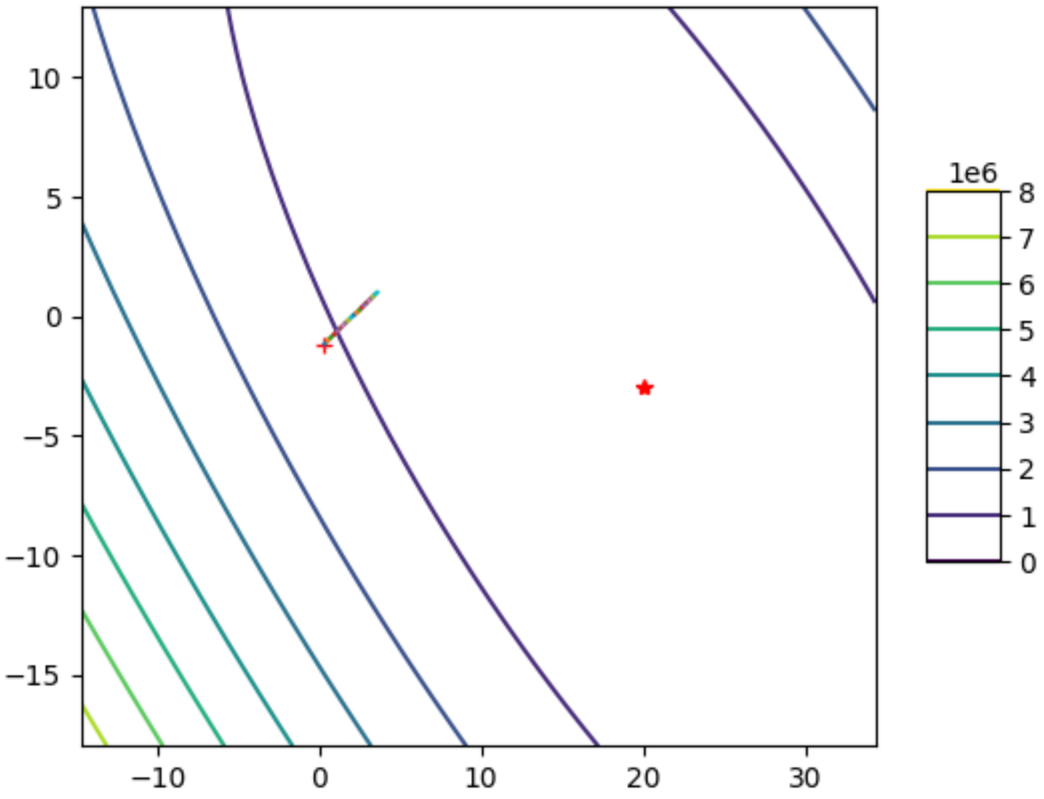
*I tried it with stochastic gradient decent and the results made me curious ...*

*Hint: I am not shure wheather you interpret the size of the mini batch as a hyper-parameter. Here, I didn't. So this is none of the approaches you wanted me to implement. Anyway, this gives a hint to the size of the learning rate that should be considered for the other approaches. In my opinion, the size of the mini batch is indeed a hyper-parameter. But unfortunately this is limited by the memory space and the size of the input data. Hence, we are not fully free in setting it.*

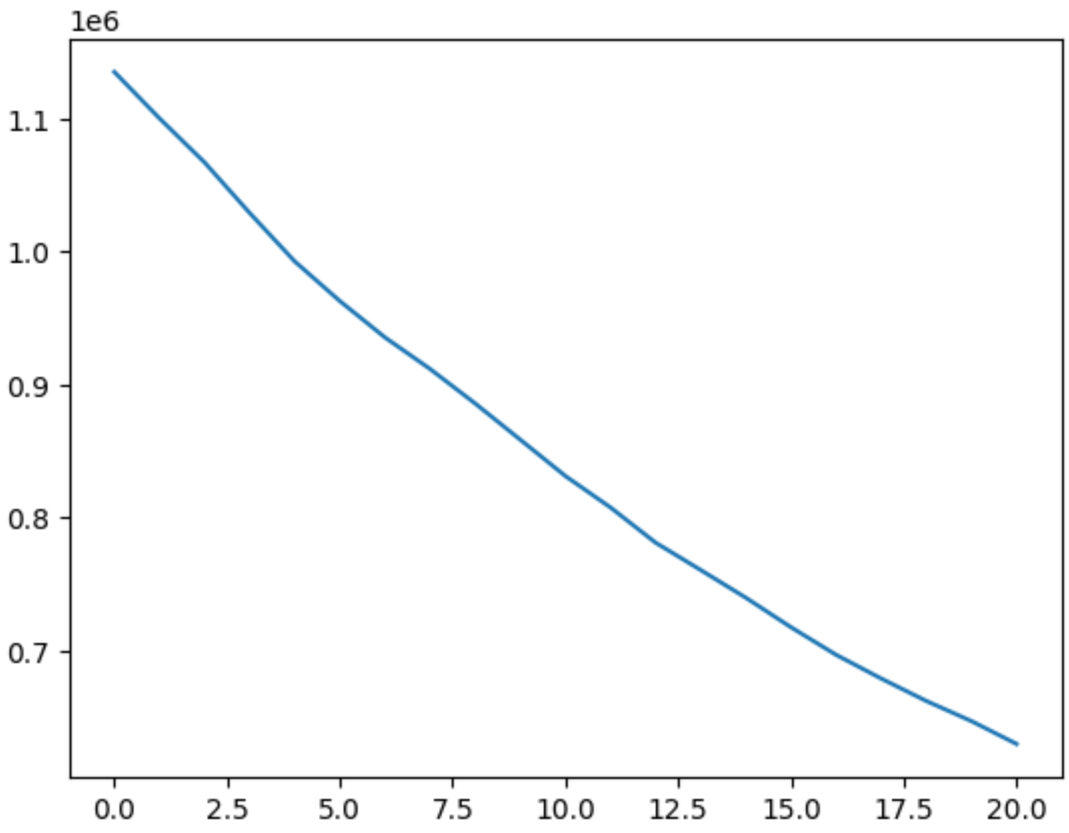
In [ ]:
```
def stochastic_grad_desc_mse(K, ws, learning_eps, loss, grad_loss, N, verbose):
    batch_size = int(N*0.01)
    hist = np.zeros((K+1))
    hist[0] = loss(ws)
    for k in range(K):
        randices = np.random.choice(np.arange(0, N), size=batch_size, replace=False
        grad_ws = grad_loss(ws,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

*Using the same learning rate, the fitting will not converge after 20 steps. So it seems that the gradient of the loss for a mini batch is smaller than for all training data.*

In [ ]:
```
np.random.seed(42)
plot3d(f, A, B, False)
plt.plot(a10, a20,'*r')
plt.plot(ws0[0], ws0[1],'+r')

# SGD
grad_loss2 = lambda ws, randinces: grad_mse(ws, m1, gradients1, XX[randinces, :], Y
learning_eps = 0.00000006
[ws, history] = stochastic_grad_desc_mse(K, ws0, learning_eps, mse1, grad_loss2, le
```

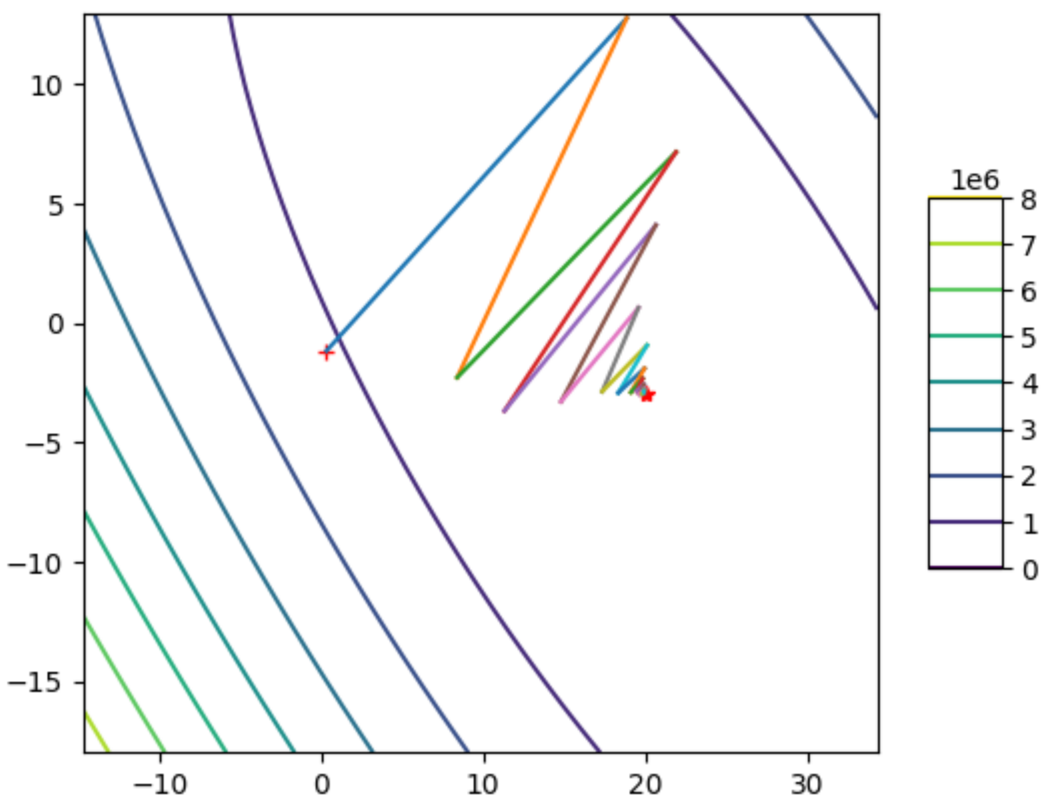


In [ ]:
```
plt.plot(range(len(history)),history)
plt.show()
```



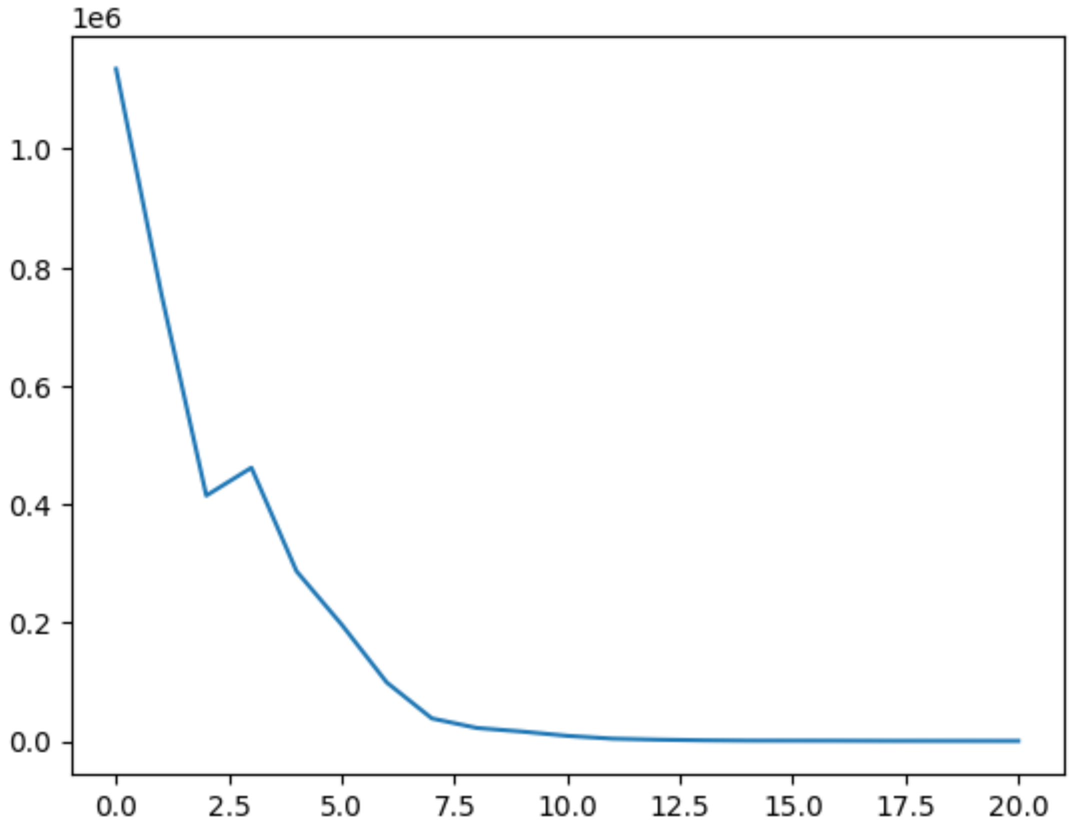
*Therefore, I used another learning rate of 6e-6 instead of 6e-8.*

```
In [ ]: np.random.seed(42)
        plot3d(f, A, B, False)
        plt.plot(a10, a20,'*r')
        plt.plot(ws0[0], ws0[1],'+r')

        # SGD
        learning_eps = 0.000006
        [ws, history] = stochastic_grad_desc_mse(K, ws0, learning_eps, mse1, grad_loss2, le
```



*Now the fitting converges after approx. $k = 11$ steps. However, here were fewer training data used compare to the first approach. Hence, the computational effort is lower.*

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



# *First approach with two hyper-parameters*

*Now I start with the approaches using at least two hyper-parameters.*

*The first optimization strategy I choosed is Stochastic Gradient Decent with adaptive learning rate. This approach works with two hyperparameters, i.e. the learning rate $\epsilon$ and the adaption factor of the learning rate $\alpha$.*

## SGD with adaptive learning rate

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

In [ ]:
```python
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 [ ]:
```python
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)
```

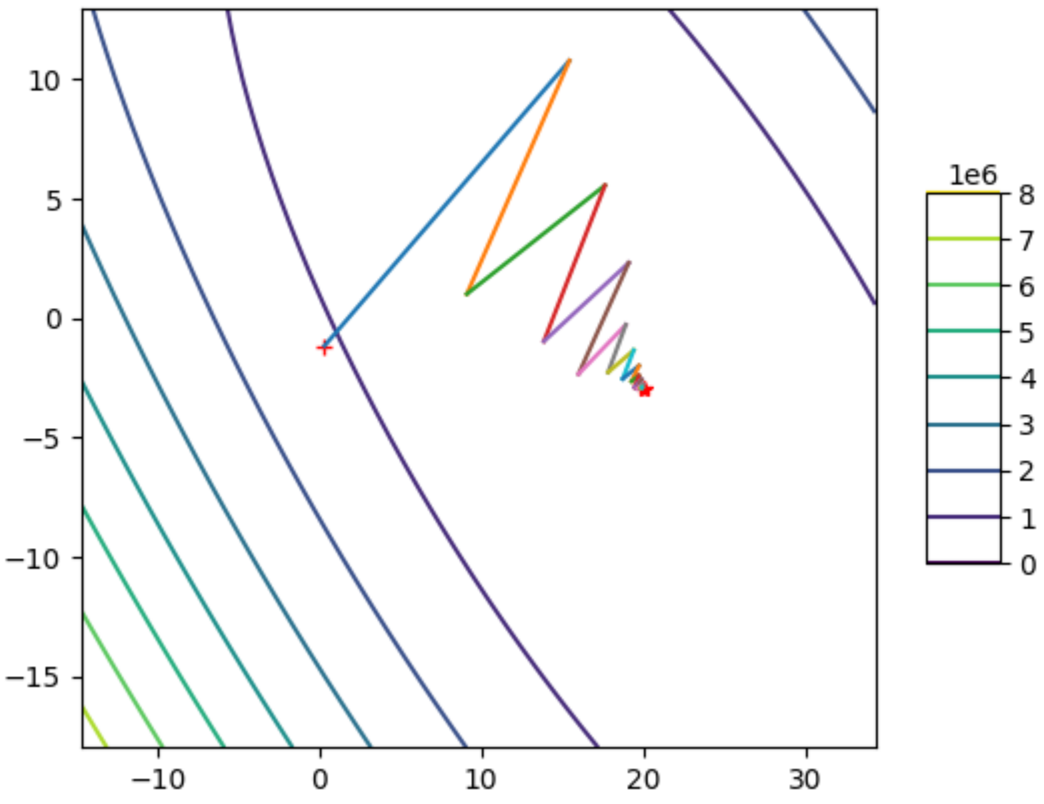
```
{'learning_eps': 6e-06, 'alpha': 1e-05}
109.2116509274781
```

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

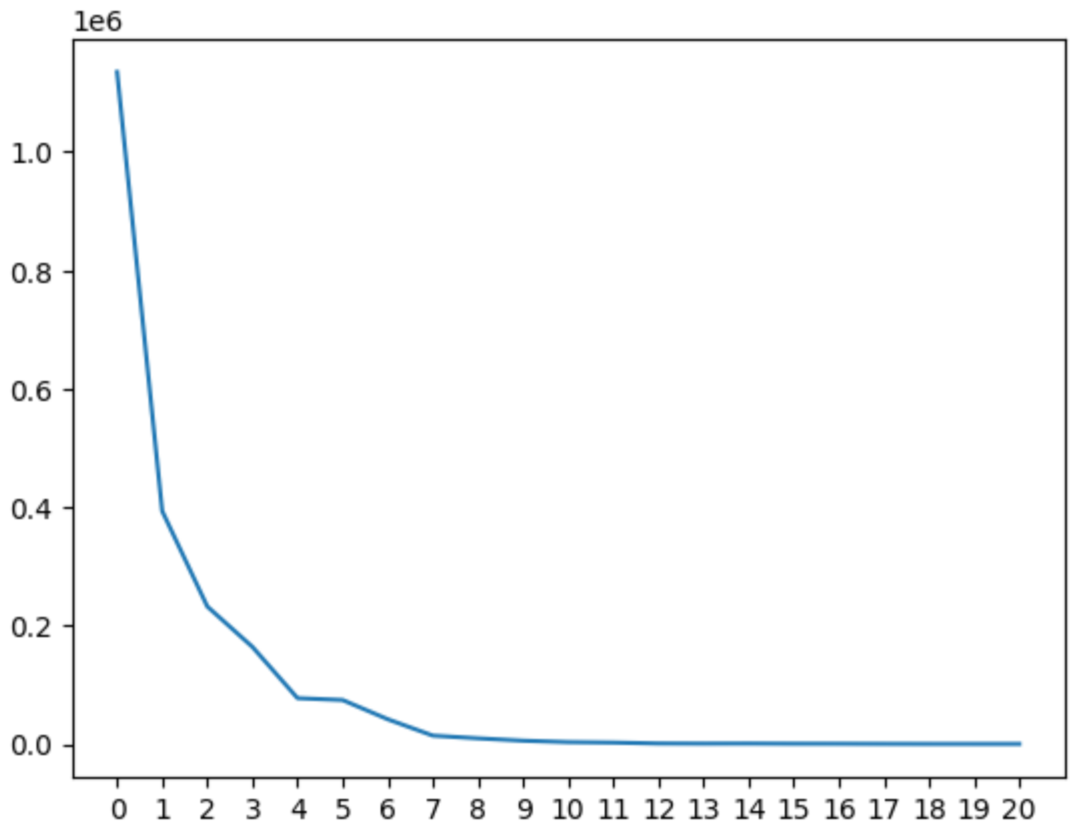
- $\varepsilon = 6e - 6$
- $\alpha = 0.00001$

*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()
```



### *Interpretation of SGD with adaptive learning rate*

*The loss function looks indicates a rather straight forward learning of the weights. It monotonically decreases and reaches a value almost zero after 9 steps.*

*In the gradient plot, one can see that the steps get smaller ans smaller, which could be due to the calculated gradients beeing smaller, but also to the smaller learning rate in each step.*

*Compared to the approach without adaptive learning rate, this resulted in a more direct moving towards the minimum*

*However, I could have done the grid search on a more detailed base. Additionally, I want to notice that the grid search is based on the loss as a score. That gives the hyper-parameters that are best for the model to find the 'best' minimum. But it does not ensure that the minimum is found in a rather straight forward way as we saw in the notebooks shown in the course.*

## *Second approach with two hyper-parameters*

*I decided to choose SDG with momentum as the second approach. This approach comes with two hyper-parameters, i.e. the learning rate $\varepsilon$ and the mass $m$ used to calculate the momentum.*

## SGD with momentum

The gradient can be understood as a velocity at which we move towards the optimum. In this analogy, momentum $p$ is introduced as the velocity $v$ (gradient) times mass $m$, a new hyper-parameter of the algorithm. The velocity is set to the average of past gradients (with importance of past velocities decaying exponentially). The initial velocity $v_0$ is the initial gradient.

**OBS!** The velocity (earlier gradient vectors) and the current gradient vector point "uphill", i.e, into the inverse direction of the expected minimum. They should, hence, be **both** subtracted from the current parameters.

In [ ]:
```
def stochastic_grad_desc_mse_with_momentum(K, ws, learning_eps, loss, grad_loss, N,
    batch_size = int(N*0.01)
    hist = np.zeros((K+1))
    hist[0] = loss(ws)
    v = 0
    for k in range(K):
        randices = np.random.choice(np.arange(0, N), size=batch_size, replace=False
        grad_ws = grad_loss(ws, randices)
        v = (v+grad_ws)/2
        old_ws = ws
        ws = old_ws - v * mass - 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
```

*Now I performed the oridinary grid search again*

In [ ]:
```
params = np.linspace(1/10*6e-6, 11/10*6e-6, 20)

param_grid = {
    'learning_eps': params.tolist(),
    'mass': params.tolist()
}

best_score = 10000000
best_params = None

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

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

print(best_params)
print(best_score)
```

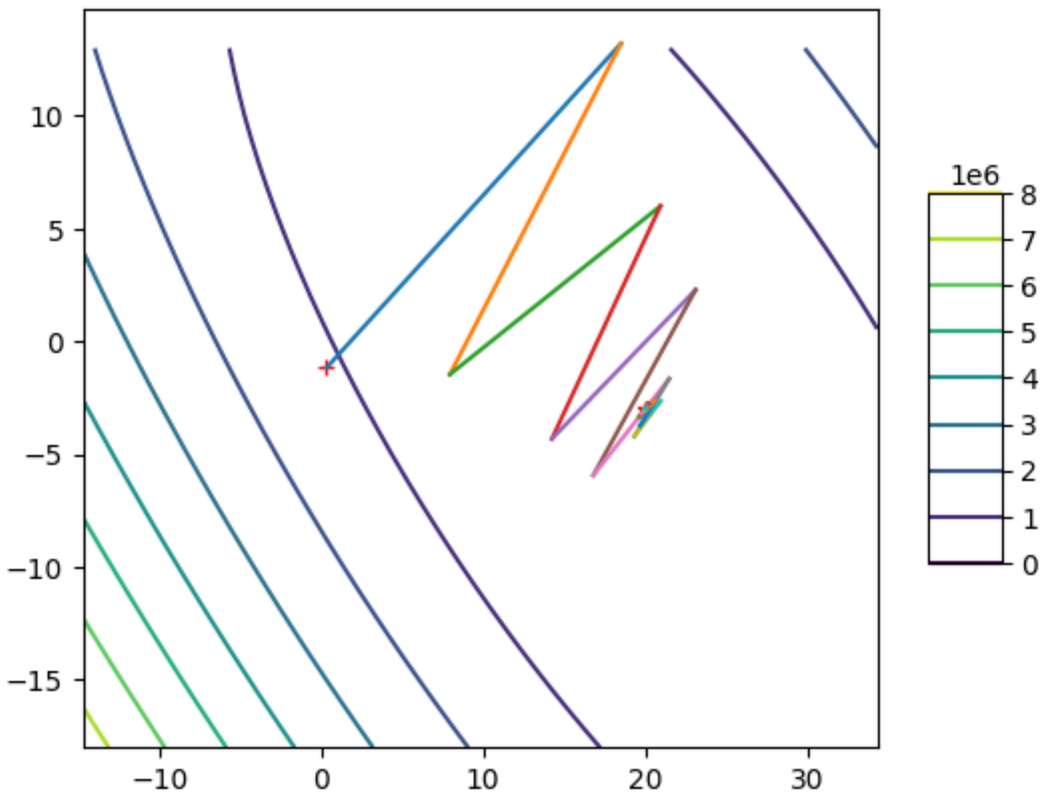
```
{'learning_eps': 4.073684210526316e-06, 'mass': 6.28421052631579e-06}
100.78314613284985
```

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

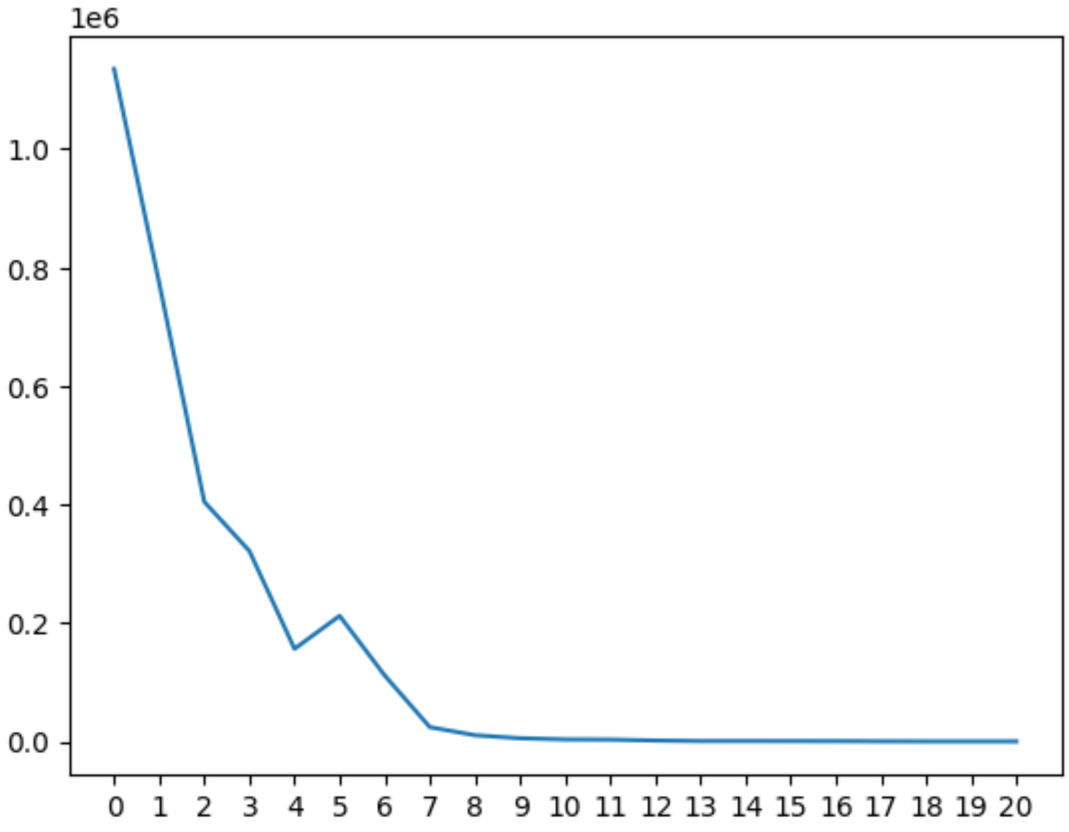
- $\varepsilon = 4.073684210526316 * 10^{-6}$
- $m = 6.28421052631579 * 10^{-6}$

*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, history2] = stochastic_grad_desc_mse_with_momentum(K, ws0, best_params['learni
```



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



### *Interpretation of SGD with momentum*

*This loss function does not monotonically decrease, since there was a increasing mse in step 5. Here the gradient pointed into a wrong direction and the step was a little bit to far, due to the gained momentum from the previous steps.*

*Looking at the gradient plot, it seems that the gradients first point into directions that led the gradient decent move more horizontal over the valley where the minimum is located. When it crosses the minimum, the loss increased (step 5) and the further gradients pointed downwards the valleym before the gradient decent converges against zero. This also let me assume, that the valley where the minimum is localted is quite narrow.*

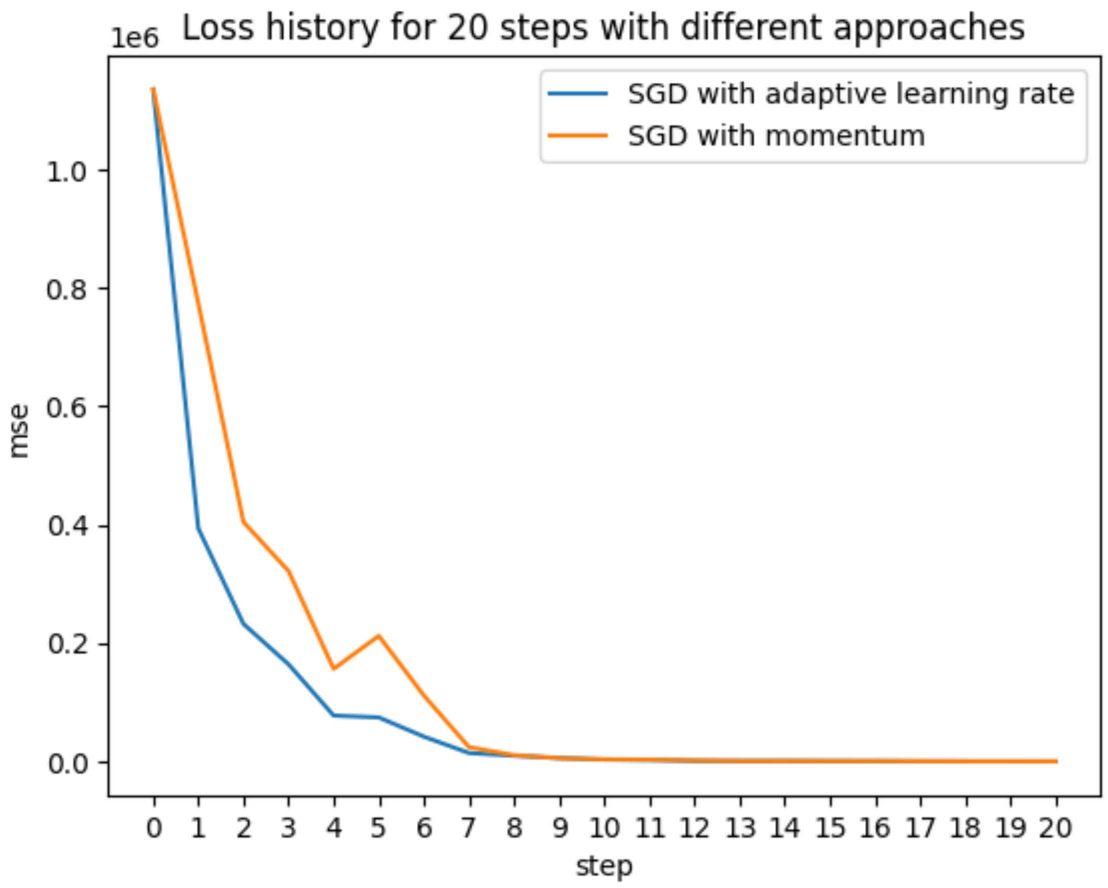
*Anyway, also this approach converges after 9 steps.*

*However, I have to notice that the search space of the parameters was quite larger than in the previous approach.*

## *Comparison*

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

```
In [ ]: plt.plot(range(len(history1)), history1, label='SGD with adaptive learning rate')
        plt.plot(range(len(history2)), history2, label='SGD with momentum')
        plt.title('Loss history for 20 steps with different approaches')
        plt.legend()
        plt.ylabel('mse')
        plt.xlabel('step')
        plt.xticks(range(len(history2)))
        plt.show()
```



## *Interpretation*

*One can see that both approaches converge after approximately 9 steps. However, compared to the SGD with adaptive learning rate the SGD with momentum starts flatter and went steeper (in both directions) after 3 steps, before it converges. This could be due to the calulated gradients of the reached points, but also because of the adapted learning rate in the SGD with adaptive learning rate approach, which make the trajectory of the loss function from SGD with adpative learning rate getting flatter and flatter*

*Additionally, SGD with momentum shows an increasing loss in step 5, whereas the change of the loss of the other approach is quite flat but still negative. So the gradient of the momentum appraoch pointed into a wrong direction and the step was a little bit to far probalbly caused by the gained momentum from the previous steps.*

*In the end, both approaches led to the minimum we aimed for in the same amount of steps.*