Learn an XOR Neural Network using gradient-based optimization

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1 Learn an XOR Neural Network using gradient-based optimization

1.1 Steps

1. Setting the scene
2. Model 1: linear, one layer, no activation function
3. Model 2: almost linear, one layer, sigmoid activation function
4. Model 3: one hidden layer with linear and one output layer with sigmoid activation
5. Model 4: one hidden layer with relu and one output layer with sigmoid activation
6. Comparison with Model 4 learned with Tensorflow

1.2 Setting the scene

All models m_i follow the standard Neural Network architecture: The models vary in the number of layers, the numbers of neurons per layer and in the activation function.

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

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

[1]:
```
%%file mse.m
function err = mse(ws,m,X,Y)
    N = length(X);
    err = 0;
    for i=1:N
        xi=X(i,:);
        yi=m(ws,xi);
        err = err + (Y(i)-yi)^2;
    end
    err = err/N;
end
```

```
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4DV660+4DV661+4DV652/Public ML Notebooks/mse.m'.
```

In other words, we find $\arg\min_{\mathbf{w},\mathbf{b}} MSE(\mathbf{w}, \mathbf{b}, m, X, Y)$. Since we implement a binary, logic function (two arguments, two values per argument), $N = 2^2 = 4$ and X, Y define the XOR function:

[2]:
```
X=[0,0;0,1;1,0;1,1]
Y=[0,1,1,0].'
```

```
X =

     0     0
     0     1
     1     0
     1     1


Y =

     0
     1
     1
     0
```

1.3 Model 1: linear, one layer, no activation function

The first model is a (too) simple linear Neural Network model. It consists of one neuron connected to the input x_1 and x_2 and an identity, i.e., no effective, activation function. The neuron and the whole model m_1 implements $m_1(\mathbf{w}, b, x) = w_1x_1 + w_2x_2 + b$.

[3]:
```
m1 = @(ws,x)(ws(1)*x(1) + ws(2)*x(2) + ws(3));
mse1 = @(ws)(mse(ws,m1,X,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. The initial bias b_0 is set to 0.

[4]:
```
in = 2;
out = 1;
limit = sqrt(6 / (in + out));
ws0 = [rand*2*limit-limit;rand*2*limit-limit;0]
```

```
ws0 =

    0.8902
```

```
    1.1478
         0
```

We are ready to assess MSE for m_1 for this initial weights setting.

[5]:
```
mse1(ws0)
```

```
ans =

    1.0468
```

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

$$
\begin{aligned}
\nabla MSE(\mathbf{w}, b) &= \left[\frac{\partial MSS(\mathbf{w}, b)}{\partial w_1}, \frac{\partial MSS(\mathbf{w}, b)}{\partial w_2}, \frac{\partial MSE(\mathbf{w}, b)}{\partial b}\right]^T \\
&= \frac{1}{4}\left[\frac{\partial \sum_{i=1}^4 (y_i - m_1(\mathbf{w}, b, x_i))^2}{\partial w_1}, \frac{\partial \sum_{i=1}^4 (y_i - m_1(\mathbf{w}, b, x_i))^2}{\partial w_2}, \frac{\partial \sum_{i=1}^4 (y_i - m_1(\mathbf{w}, b, x_i))^2}{\partial b}\right]^T \\
&= \frac{1}{4}\left[\sum_{i=1}^4 2(y_i - m_1(\mathbf{w}, b, x_i))\frac{-\partial m_1(\mathbf{w}, b, x_i)}{\partial w_1}, \sum_{i=1}^4 2(y_i - m_1(\mathbf{w}, b, x_i))\frac{-\partial m_1(\mathbf{w}, b, x_i)}{\partial w_2}, \sum_{i=1}^4 2(y_i - m_1(\mathbf{
\\
&= -\frac{1}{2}\left[\sum_{i=1}^4 (y_i - m_1(\mathbf{w}, b, x_i))\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial w_1}, \sum_{i=1}^4 (y_i - m_1(\mathbf{w}, b, x_i))\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial w_2}, \sum_{i=1}^4 (y_i - m_1(\mathbf{w}, b, x_i
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial w_j} &= \frac{\partial (\sum_{j=1}^2 w_j x_{ij}) + b}{\partial w_j} = x_{ij} \\
\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial b} &= \frac{\partial (\sum_{j=1}^2 w_j x_{ij}) + b}{\partial b} = 1
\end{aligned}
$$

We have already defined the function m_1. Let's also define the functions of the first derivative of m_1 wrt. w_1, w_2, and b resp. For the sake of generality, we keep the parameters $\mathbf{w}, b$ that are actually not needed for derivatives of this concrete model m_1.

[6]:
```
gradients1{1} = @(ws,x)(x(1));
gradients1{2} = @(ws,x)(x(2));
gradients1{3} = @(ws,x)(1);
```

The gradient of MSE can now be defined using m_1 and the first derivative of m_1 wrt. w_1, w_2, and b, resp., as parameters.

[7]:
```
%%file grad_mse.m
function grad_ws = grad_mse(ws, m, grads, X, Y)
    N = length(X);
    M = length(ws);
    grad_ws = zeros(M,1);
    for i=1:N
        xi = X(i,:);
        yi = Y(i);
        tmp = yi - m(ws,xi);
        for j=1:M
            grad_ws(j) = grad_ws(j) + tmp*grads{j}(ws,xi);
        end
    end
    grad_ws = -2/N*grad_ws;
end
```

```
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4DV660+4DV661+4DV652/Public ML Notebooks/grad_mse.m'.
```

Finally, we are ready to define the gradient descent function optimizing $\mathbf{w}, b$ by iterating over:

$$(\mathbf{w}_{k+1}, b_{k+1}) = (\mathbf{w}_k, b_k) - \varepsilon \nabla MSE(\mathbf{w}_k, b_k)$$

staring with $(\mathbf{w}_0, b_0)$.

[8]:
```
%%file grad_desc_mse.m
function [ws, history] = grad_desc_mse(K, ws, learning_eps, loss, grad_loss,␣
 ↪verbose)
    history(1) = loss(ws);
    for k = 1:K
        grad_ws = grad_loss(ws);
        old_ws = ws;
        ws= old_ws - learning_eps * grad_ws;
        if verbose
            line([old_ws(1),ws(1)],[old_ws(2),ws(2)]);
        end
        history(k+1) = loss(ws);
    end
end
```

```
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4DV660+4DV661+4DV652/Public ML Notebooks/grad_desc_mse.m'.
```
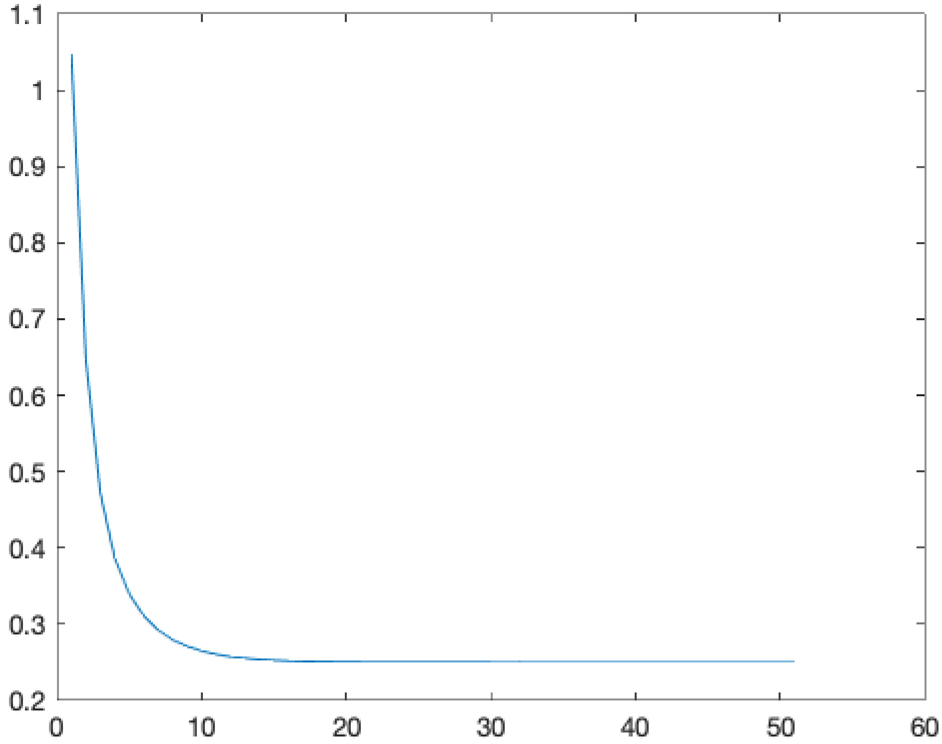

[9]:
```
grad_loss = @(ws)(grad_mse(ws, m1, gradients1, X, Y));
K = 50;
```

```
learning_eps = 0.5;
[ws, history] = grad_desc_mse(K, ws0, learning_eps, mse1, grad_loss, false)
```

```
ws =

    0.0002
    0.0002
    0.4998


history =

  Columns 1 through 7

    1.0468    0.6465    0.4718    0.3864    0.3394    0.3108    0.2923

  Columns 8 through 14

    0.2797    0.2710    0.2648    0.2605    0.2575    0.2553    0.2538

  Columns 15 through 21

    0.2527    0.2519    0.2514    0.2510    0.2507    0.2505    0.2503

  Columns 22 through 28

    0.2502    0.2502    0.2501    0.2501    0.2501    0.2500    0.2500

  Columns 29 through 35

    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500

  Columns 36 through 42

    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500

  Columns 43 through 49

    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500

  Columns 50 through 51

    0.2500    0.2500
```

[10]:

```
plot(1:length(history),history)
```



[11]:

```
my_xor1 = @(x1, x2)(round(ws(1)*x1 + ws(2)*x2 + ws(3)));
for i=1:4
    fprintf("my_xor1(%d,%d)=%d\n", X(i,1),X(i,2), my_xor1(X(i,1),X(i,2)))
end
```

```
my_xor1(0,0)=0
my_xor1(0,1)=0
my_xor1(1,0)=0
my_xor1(1,1)=1
```

[12]:

```
%%file accuracy.m
function a = accuracy(X,Y,f)
    correct = 0;
    for i=1:length(X)
        y = f(X(i,1),X(i,2));
        if y==Y(i)
```

```
            correct = correct +1;
        else
            fprintf("f(%d,%d)=%d, but should be %d\n", X(i,1),X(i,2), y, Y(i))
        end
    end
    a=correct/length(X);
end
```

```
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4DV660+4DV661+4DV652/Public ML Notebooks/accuracy.m'.
```
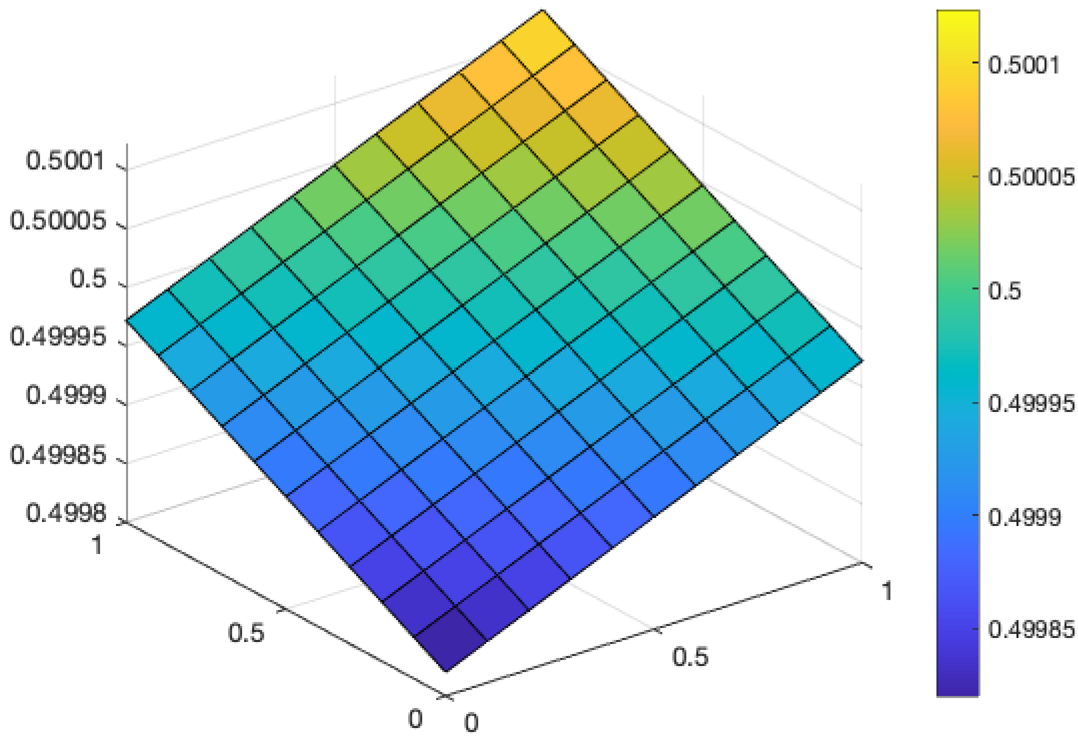

[13]:

```
a=accuracy(X,Y,my_xor1)
```

```
f(0,1)=0, but should be 1
f(1,0)=0, but should be 1
f(1,1)=1, but should be 0

a =

    0.2500
```

[14]:

```
f = @(x1, x2)(ws(1)*x1 + ws(2)*x2+ws(3));
[A,B] = meshgrid(0:0.1:1,0:0.1:1);
plot3d(f, A, B, true)
```



1.4 Model 2: linear, one layer, sigmoid activation function

The second model is still a (too) simple Neural Network model. As model m_1, it consists of one neuron connected to the input x_1 and x_2 but it uses a sigmoid activation function $s(x) = \frac{1}{1+e^{-x}}$. The cell body still implements $m_1(\mathbf{w}, b, x) = w_1x_1 + w_2x_2 + b$, the whole model m_2 implements:

$$m_2(\mathbf{w}, b, x) = \frac{1}{1 + e^{-m_1(\mathbf{w},b,x)}}$$

Note that we just plug in m_1 into m_2 and m_2 into the loss function MSE to obtain the new composite model and loss functions.

[15]:
```
s = @(x)(1.0 / (1.0 + exp(-x)));
m2 = @(ws,x)(s(m1(ws,x)));
mse2 = @(ws)(mse(ws,m2,X,Y));
```

```
s =

  function_handle with value:
```

```
    @(x)(1.0/(1.0+exp(-x)))


m2 =

  function_handle with value:

    @(ws,x)(s(m1(ws,x)))


mse2 =

  function_handle with value:

    @(ws)(mse(ws,m2,X,Y))
```

As we use the same initialization, we can assess MSE for m_2 and this initial weights setting.

[16]:
```
mse2(ws0)
```

```
ans =

    0.2939
```

For model m_2, the gradient of $MSE(\mathbf{w}, b)$ for any $\mathbf{w}, b$ is almost identical as before. We just plug in m_2 instead of m_1 and m_2' instead of m_1':

$$\nabla MSE(\vec{w}, b) = -\frac{1}{2}\left[\sum_{i=1}^{4}(y_i - m_2(\mathbf{w}, b, x_i))\frac{\partial m_2(\mathbf{w}, b, x_i)}{\partial w_1}, \sum_{i=1}^{4}(y_i - m_2(\mathbf{w}, b, x_i))\frac{\partial m_2(\mathbf{w}, b, x_i)}{\partial w_2}, \sum_{i=1}^{4}(y_i - m_2(\mathbf{w}, b, x_i$$

Let $s(x) = \frac{1}{1+e^{-x}}$. Then $\frac{\partial s(x)}{\partial x} = s(x)s(1-x)$, see the details here.

$$\begin{aligned}\frac{\partial m_2(\mathbf{w}, b, x_i)}{\partial \mathbf{w}, b} &= \frac{\partial s(m_1(\mathbf{w}, b, x_i))}{\partial \mathbf{w}, b} \\ &= s(m_1(\mathbf{w}, b, x_i))s(1 - m_1(\mathbf{w}, b, x_i))\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial \mathbf{w}, b}\end{aligned}$$

We can plug in the function m_1 and the first derivative of m_1 wrt. w_1, w_2, and b, resp., as computed before.

$$\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial w_j} = \frac{\partial (\sum_{j=1}^{2} w_j x_{ij}) + b}{\partial w_j} = x_{ij}$$
$$\frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial b} = \frac{\partial (\sum_{j=1}^{2} w_j x_{ij}) + b}{\partial b} = 1$$

We have already defined the function m_1, the functions of the first derivative of m_1 wrt. w_1, w_2, and b, resp, and the sigmoid activation function f. The gradient calculation depends of these functions and the gradient descent method does not change either. We just need to pulg together the new neural network:

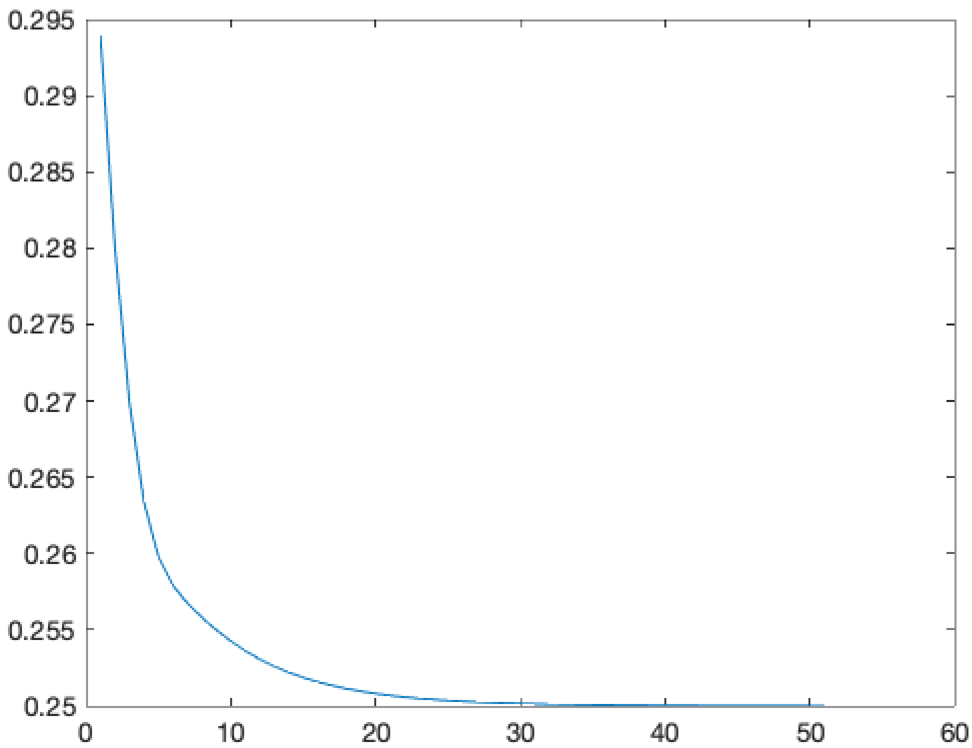
[17]:
```
gradients2{1} = @(ws,x)(s(m1(ws,x))*s(1-m1(ws,x))*gradients1{1}(ws,x));
gradients2{2} = @(ws,x)(s(m1(ws,x))*s(1-m1(ws,x))*gradients1{2}(ws,x));
gradients2{3} = @(ws,x)(s(m1(ws,x))*s(1-m1(ws,x))*gradients1{3}(ws,x));
```

[18]:
```
grad_loss = @(ws)(grad_mse(ws, m2, gradients2, X, Y));
K = 50;
learning_eps = 2;
[ws, history] = grad_desc_mse(K, ws0, learning_eps, mse2, grad_loss, false)
```

```
ws =

   -0.0001
    0.0204
   -0.0131


history =

  Columns 1 through 7

    0.2939    0.2800    0.2699    0.2634    0.2598    0.2579    0.2567

  Columns 8 through 14

    0.2558    0.2550    0.2543    0.2536    0.2531    0.2526    0.2522

  Columns 15 through 21

    0.2519    0.2516    0.2513    0.2511    0.2510    0.2508    0.2507

  Columns 22 through 28

    0.2506    0.2505    0.2504    0.2504    0.2503    0.2503    0.2502
```

```
  Columns 29 through 35

    0.2502    0.2502    0.2501    0.2501    0.2501    0.2501    0.2501

  Columns 36 through 42

    0.2501    0.2501    0.2500    0.2500    0.2500    0.2500    0.2500

  Columns 43 through 49

    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500    0.2500

  Columns 50 through 51

    0.2500    0.2500
```

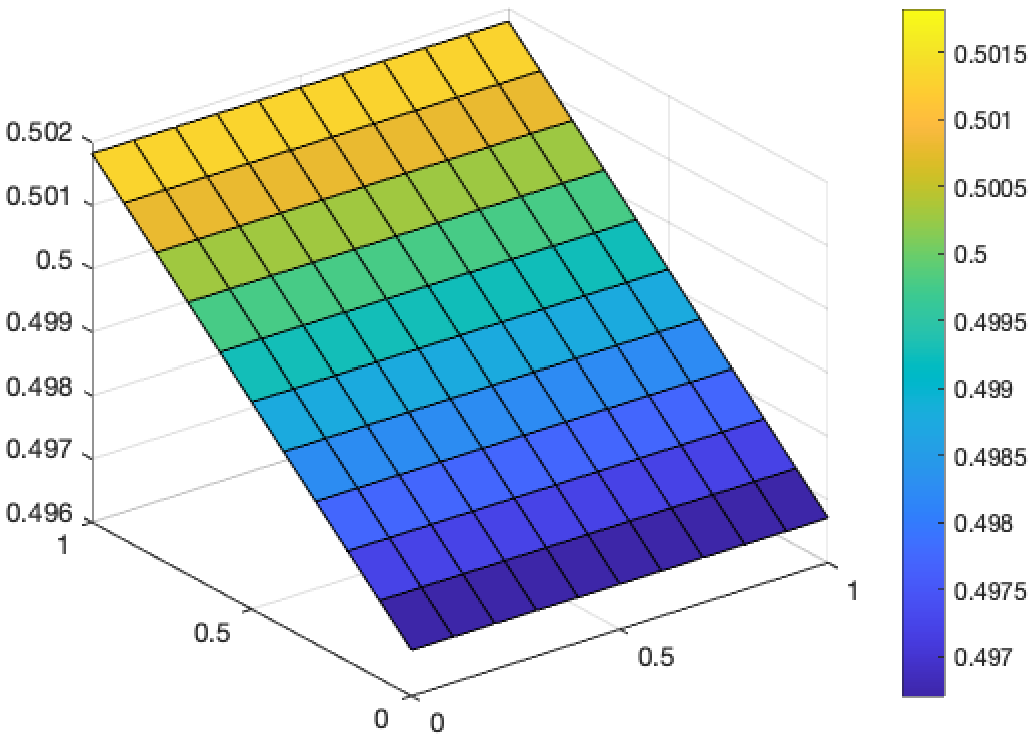
[19]:
```
plot(1:length(history),history)
```



[20]:
```
my_xor2 = @(x1, x2)(round(s(ws(1)*x1 + ws(2)*x2 + ws(3))));
for i=1:4
    fprintf("my_xor2(%d,%d)=%d\n", X(i,1),X(i,2), my_xor2(X(i,1),X(i,2)))
end
a=accuracy(X,Y,my_xor2)
```

```
my_xor2(0,0)=0
my_xor2(0,1)=1
my_xor2(1,0)=0
my_xor2(1,1)=1
f(1,0)=0, but should be 1
f(1,1)=1, but should be 0

a =

    0.5000
```

[21]:
```
f = @(x1, x2)(s(ws(1)*x1 + ws(2)*x2 + ws(3)));
[A,B] = meshgrid(0:0.1:1,0:0.1:1);
plot3d(f, A, B, true)
```



Not much changes as the co-domain of m_1 is just in the domain of the sigmoid activation function s where it is almost linear.

1.5 Model 3: one hidden layer with linear and one output layer with sigmoid activation

The third model adds a hidden layer of 32 neurons with linear activation function. Each of these neurons uses the three parameters w_1, w_2, b. As before, all parameters are captured in the parameter array `ws`. The parameters for each neuron are at different positions in this array. Let's define the model m_3 with hidden and output layers and the corresponding loss function MSE.

[22]:
```
%%file hidden_layer.m
function y = hidden_layer(ws,x,n)
    y = zeros(n,1);
    for i=1:n
        i1 = (i-1)*3+1;
        i2 = (i-1)*3+2;
        i3 = (i-1)*3+3;
        y(i) = ws(i1)*x(1)+ws(i2)*x(2)+ws(i3);%as m1 before
    end
end
```

```
Created file '/Users/wlomsi/Documents/ProjekteUni/Vorlesungen/ML
4DV660+4DV661+4DV652/Public ML Notebooks/hidden_layer.m'.
```

[23]:
```
n=32;
%weights indices for the output layer n*3+1=97:n*3+n=128
%bias index for for the output layer n*3+n+1=129
mo = @(ws,x)(dot(hidden_layer(ws,x,n),ws(n*3+1:n*3+n))+ws(n*3+n+1));
m3 = @(ws,x)(s(mo(ws,x)));
mse3 = @(ws)(mse(ws,m3,X,Y));
```

We initialize the weight vector:

[24]:
```
ws0 = zeros(n*3+n+1,1);%129
in = 2;
out = 1;
limit = sqrt(6 / (in + out));
for i=1:n
    i1 = (i-1)*3+1;
    i2 = (i-1)*3+2;
    i3 = (i-1)*3+3;
    ws0(i1) = rand*2*limit-limit;
    ws0(i2) = rand*2*limit-limit;
    ws0(i3) = 0;
end
in = n;
out = 1;
limit = sqrt(6 / (in + out));
for i=n*3+1:n*3+n
    ws0(i) = rand*2*limit-limit;
end
ws0
```

```
ws0 =

   -1.0550
    1.1692
         0
    0.3744
   -1.1383
         0
   -0.6265
    0.1326
         0
    1.2940
    1.3149
         0
```

```
-0.9684
 1.3310
      0
 1.2931
-0.0414
      0
 0.8493
-1.0129
      0
-0.2213
 1.1759
      0
 0.8265
 1.2996
      0
 0.4405
-1.3132
      0
 0.9875
 1.2275
      0
 0.5055
 0.7290
      0
 0.6877
-0.3048
      0
 0.4398
-0.9300
      0
 0.5828
-1.3242
      0
-0.6310
-1.2836
      0
-1.1395
 0.9149
      0
 0.5511
-0.5173
      0
 1.2734
-1.3168
      0
-0.1733
-0.3350
      0
```

```
 0.7510
 0.8350
      0
-0.8857
-0.0290
      0
-0.1539
 0.4138
      0
 0.5922
 0.7204
      0
-0.6335
 0.5083
      0
 0.4387
-0.9543
      0
-1.0776
-0.0046
      0
 1.3004
-0.4515
      0
 0.2412
-0.7812
      0
 0.7107
-0.6927
      0
 0.0168
 0.5631
      0
 1.1056
 1.2991
      0
 0.0403
-0.3082
-0.2991
-0.2068
 0.2906
-0.2095
 0.2680
-0.2187
 0.3661
-0.1279
-0.2587
-0.2123
```

```
 0.0990
-0.0228
-0.1265
 0.2821
 0.0727
 0.0424
 0.3558
-0.1826
 0.2193
 0.2164
-0.1020
 0.0578
-0.3617
-0.3804
 0.0263
 0.2381
 0.3701
-0.3156
 0.0587
-0.0261
      0
```

We are ready to compute the initial loss:

[25]:
```
mse3(ws0)
```

```
ans =

    0.2553
```

Even for model the m_3 the gradient of $MSE(\mathbf{ws}_o, \mathbf{ws}_h)$ for any weight $\mathbf{ws}_o, \mathbf{ws}_h$ of the output and hidden layers, resp., is almost identical as before. We just plug in m_3 instead of m_2 and m_3' instead of m_2':

$$
\begin{aligned}
\nabla MSE(\mathbf{ws}_o, \mathbf{ws}_h) &= -\frac{1}{2}\left[\sum_{i=1}^{4}(y_i - m_3(\mathbf{ws}_o, \mathbf{ws}_h)\frac{\partial m_3(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial \mathbf{ws}_o, \mathbf{ws}_h}\right]^T \\
\frac{\partial m_3(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial(\mathbf{ws}_o, \mathbf{ws}_h)} &= \frac{\partial s(m_o(\vec{ws}_o, \vec{ws}_h, x_i))}{\partial(\mathbf{ws}_o, \mathbf{ws}_h)} \\
&= s(m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i))s(1 - m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i))\frac{\partial m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial(\mathbf{ws}_o, \mathbf{ws}_h)} \\
\frac{\partial m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial(\mathbf{ws}_o, \mathbf{ws}_h)} &= \frac{\partial \sum_{k=1}^{n}(m_1(\mathbf{ws}_{h,3(k-1)+1:2}, \mathbf{ws}_{h,3(k-1)+3}, x_i)\mathbf{ws}_{o,k}) + \mathbf{ws}_{o,n+1}}{\partial(\mathbf{ws}_o, \mathbf{ws}_h)}
\end{aligned}
$$

The term $\mathbf{ws}_{o,k}$ selects the k weights of the output layer and the term $\mathbf{ws}_{o,k+1}$ selects the bias b from the vector $\mathbf{ws}_o$. The term $\mathbf{ws}_{h,3(k-1)+1:2}$ selects the two weights $\mathbf{w}_{k,1}$ and $\mathbf{w}_{k,2}$ of the k-th neuron in the hidden layer, and the term $\mathbf{ws}_{h,3(k-1)+3}$ selects the k-th bias $\mathbf{b}_k$ from the vector $\mathbf{ws}_h$.

The gradients wrt. the parameters of the hidden layer are

$$\frac{\partial m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial \mathbf{ws}_{h,3(k-1)+j}} = \begin{cases} \frac{\partial m_1(\mathbf{w}_k, b_k, x_i)}{\partial \mathbf{w}_{k,j}} \mathbf{ws}_{o,k}, & \text{if } j = 1,2 \\ \frac{\partial m_1(\mathbf{w}_k, b_k, x_i)}{\partial b_k} \mathbf{ws}_{o,k}, & \text{if } j = 3 \end{cases}$$

Since the cell function of the hidden layer is m_1, we can plug in the first derivative of m_1 wrt. w_1, w_2, and b, resp., as computed before.

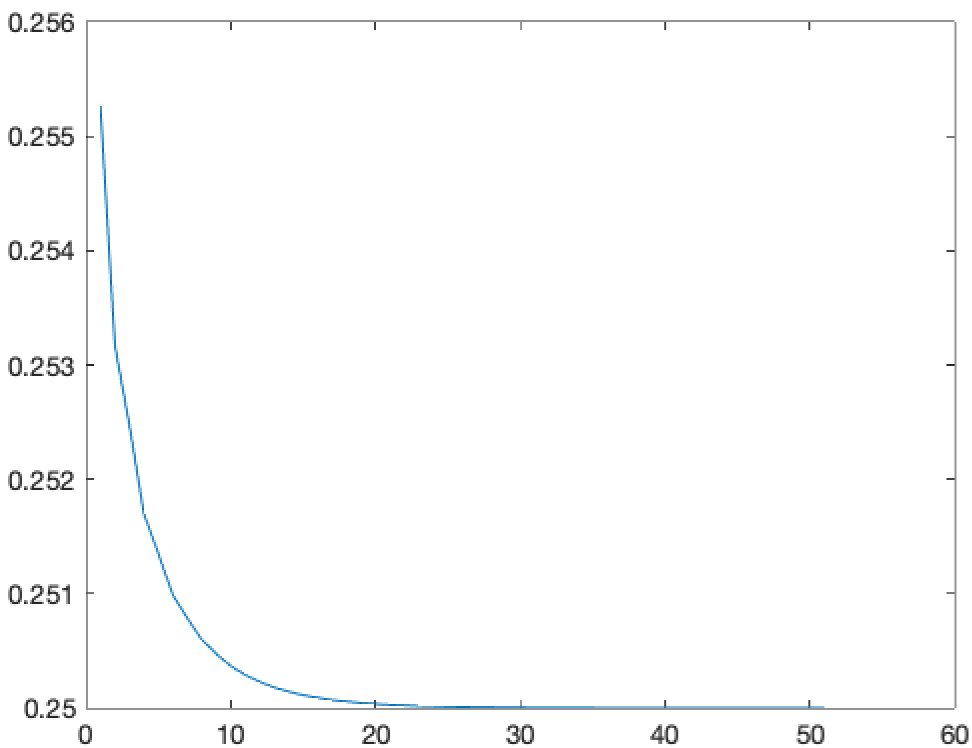
$$\begin{aligned} \frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial w_j} &= \frac{\partial (\sum_{j=1}^{2} w_j x_{ij}) + b}{\partial w_j} = x_{ij} \\ \frac{\partial m_1(\mathbf{w}, b, x_i)}{\partial b} &= \frac{\partial (\sum_{j=1}^{2} w_j x_{ij}) + b}{\partial b} = 1 \end{aligned}$$

The gradients wrt. the weights and the bias, resp., of the output layer are

$$\begin{aligned} \frac{\partial m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial \mathbf{ws}_{o,k}} &= m_1(\vec{w_k}, b_k, x_i) \\ \frac{\partial m_o(\mathbf{ws}_o, \mathbf{ws}_h, x_i)}{\partial \mathbf{ws}_{o,n+1}} &= 1 \end{aligned}$$

[26]:
```
%parameters (weights and bias) hidden layer
for k=1:n
    i1 = 3*(k-1)+1;
    i2 = 3*(k-1)+2;
    i3 = 3*(k-1)+3;
    gradients3{i1} = @(ws,x)(s(mo(ws,x))*s(1-mo(ws,x))*x(1)*ws(3*n+k));␣
 ↪%gradients1{1}=x(1)
    gradients3{i2} = @(ws,x)(s(mo(ws,x))*s(1-mo(ws,x))*x(2)*ws(3*n+k));␣
 ↪%gradients1{2}=x(2)
    gradients3{i3} = @(ws,x)(s(mo(ws,x))*s(1-mo(ws,x))*ws(3*n+k));␣
 ↪%gradients1{3}=1
    model1{k} = @(ws,x)(ws(i1)*x(1)+ws(i2)*x(2)+ws(i3));
end
%weights output layer
k=1;
for i=3*n+1:3*n+n
    gradients3{i} = @(ws,x)(s(mo(ws,x))*s(1-mo(ws,x))*model1{k}(ws,x));
    k=k+1;
end
%bias output layer
gradients3{3*n +1} = @(ws,x)(s(mo(ws,x))*s(1-mo(ws,x)));
```

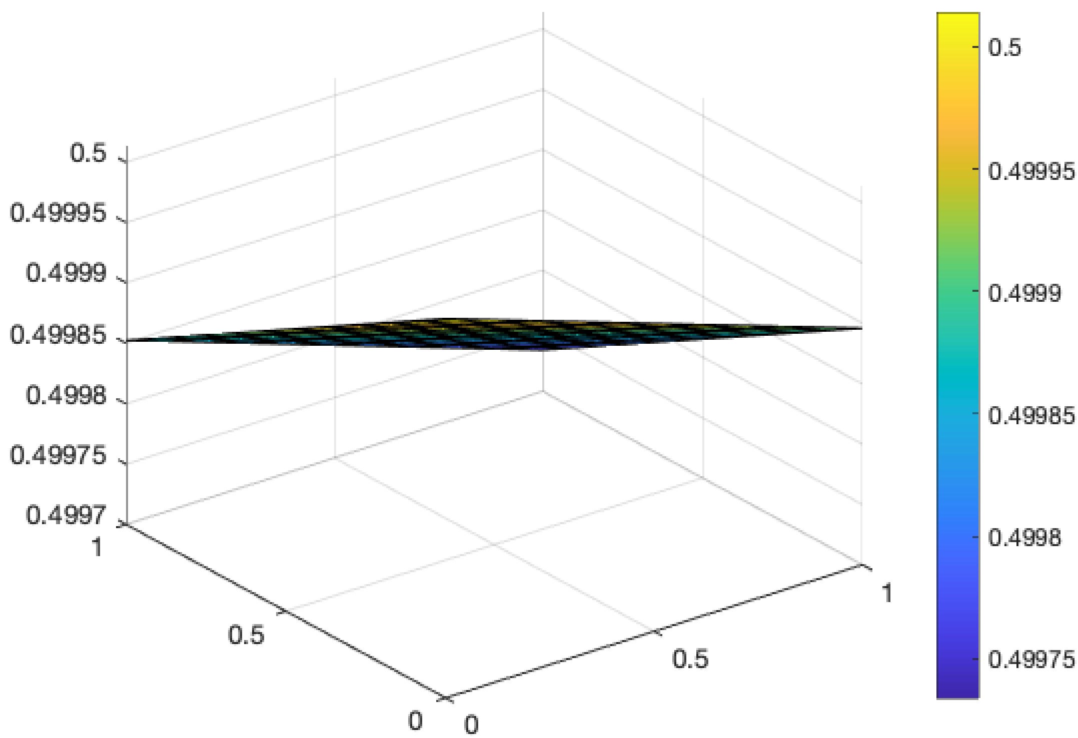
[27]:
```
grad_loss = @(ws)(grad_mse(ws, m3, gradients3, X, Y));
K = 50;
learning_eps = 0.5;
[ws, history] = grad_desc_mse(K, ws0, learning_eps, mse3, grad_loss, false);
plot(1:length(history),history)
```



[28]:
```
my_xor3 = @(x1, x2)(round(m3(ws,[x1,x2])));
for i=1:4
    fprintf("my_xor3(%d,%d)=%d\n", X(i,1),X(i,2), my_xor3(X(i,1),X(i,2)))
end
a=accuracy(X,Y,my_xor3)
f = @(x1, x2)(m3(ws,[x1,x2]));
[A,B] = meshgrid(0:0.1:1,0:0.1:1);
plot3d(f, A, B, true)
```

```
my_xor3(0,0)=1
my_xor3(0,1)=0
my_xor3(1,0)=0
```

```
my_xor3(1,1)=0
f(0,0)=1, but should be 0
f(0,1)=0, but should be 1
f(1,0)=0, but should be 1

a =

    0.2500
```



1.6 Model 4: one hidden layer with relu and one output layer with sigmoid activation

The final model uses the Rectified Linear Unit (ReLU) activation function $r(x) = \max(0, x)$ in the hidden layer. Hence, the hidden layer neurons compute $\max(0, w_1x_1 + w_2x_2 + b) = \max(0, m_1(\vec{w}, b, x))$. We can easily change the hidden layer function accordingly.

[29]:
```
hidden_layer_4 = @(ws,x,n)(max(0,hidden_layer(ws,x,n)));
mo4 = @(ws,x)(dot(hidden_layer_4(ws,x,n),ws(n*3+1:n*3+n))+ws(n*3+n+1));
m4 = @(ws,x)(s(mo4(ws,x)));
```

```
mse4 = @(ws)(mse(ws,m4,X,Y));
```

The network structure does not change, hence, the initialization remains the same as well. We can directly compute the initial loss:

[30]:
```
mse4(ws0)
```

```
ans =

    0.2284
```

No surprise it is the same as for model m_3 as all weights and all input is positive.

As for the model m_4 itself, we need to subsitute $m_1(\mathbf{w}, b, x)$ with $r(\mathbf{w}, b, x) = \max(0, m_1(\mathbf{w}, b, x))$ and $m_1'(\mathbf{w}, b, x)$ with $r'(m_1(\mathbf{w}, b, x))m_1'(\mathbf{w}, b, x)$.

$$r'(z) = \begin{cases} 0, & \text{if } z < 0 \\ 1, & \text{if } z > 0 \end{cases}$$

Note that $r'(z)$ is undefined in $z = 0$, since its left and right derivative are not equal for $z = 0$. In practice , we pick $r'(0) = 0$ as Tensorflow does. Consequently:

$$r'(m_1(\mathbf{w}, b, x))m_1'(\mathbf{w}, b, x) = \begin{cases} 0, & \text{if } m_1(\mathbf{w}, b, x) \leq 0 \\ m_1'(\mathbf{w}, b, x), & \text{if } m_1(\mathbf{w}, b, x) > 0 \end{cases}$$

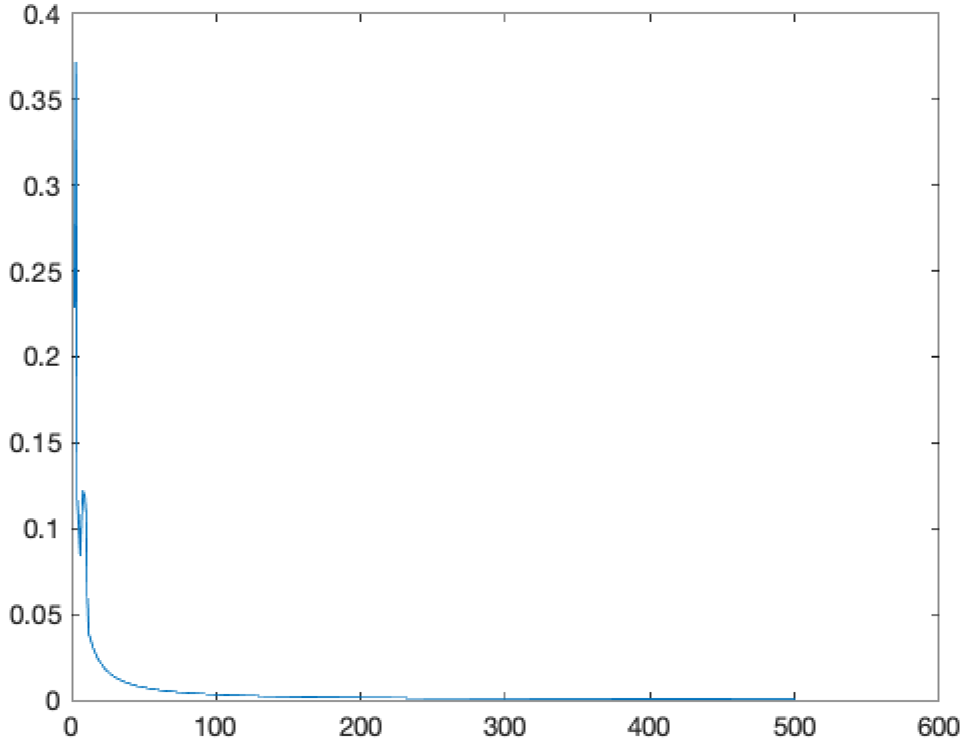
[31]:
```
%%file ite.m
function res = ite(cond, tc, fc)
    if (cond)
        res = tc;
    else
        res = fc;
    end
end
```

```
Created file '/Users/wlomsi/Documents/ProjekteUni/Vorlesungen/ML
4DV660+4DV661+4DV652/Public ML Notebooks/ite.m'.
```

[32]:
```
%parameters (wights and bias) hidden layer
for k=1:n
    i1 = 3*(k-1)+1;
    i2 = 3*(k-1)+2;
    i3 = 3*(k-1)+3;
    model1{k} = @(ws,x)(max(0,ws(i1)*x(1)+ws(i2)*x(2)+ws(i3)));
```

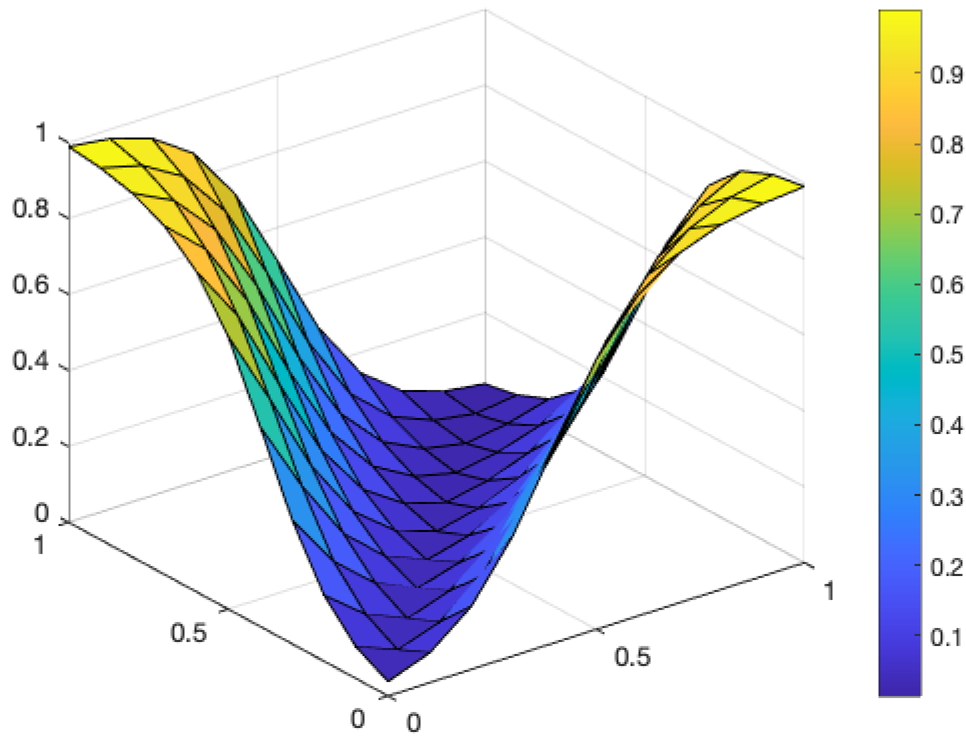
```
    gradients4{i1} =␣
↪@(ws,x)(s(mo4(ws,x))*s(1-mo4(ws,x))*ite(model1{k}(ws,x)<=0,0,x(1))*ws(3*n+k));
↪
    gradients4{i2} =␣
↪@(ws,x)(s(mo4(ws,x))*s(1-mo4(ws,x))*ite(model1{k}(ws,x)<=0,0,x(2))*ws(3*n+k));
↪
    gradients4{i3} =␣
↪@(ws,x)(s(mo4(ws,x))*s(1-mo4(ws,x))*ite(model1{k}(ws,x)<=0,0,1)*ws(3*n+k));
end
%weights output layer
k=1;
for i=3*n+1:3*n+n
    gradients4{i} = @(ws,x)(s(mo4(ws,x))*s(1-mo4(ws,x))*max(0,model1{k}(ws,x)));
    k=k+1;
end
%bias output layer
gradients4{3*n+n +1} = @(ws,x)(s(mo4(ws,x))*s(1-mo4(ws,x)));
```

[33]:
```
grad_loss = @(ws)(grad_mse(ws, m4, gradients4, X, Y));
K =500;
learning_eps = 1.5;
[ws, history] = grad_desc_mse(K, ws0, learning_eps, mse4, grad_loss, false);
plot(1:length(history),history)
```



[34]:
```
my_xor4 = @(x1, x2)(round(m4(ws,[x1,x2])));
for i=1:4
    fprintf("my_xor4(%d,%d)=%d\n", X(i,1),X(i,2), my_xor4(X(i,1),X(i,2)))
end
a=accuracy(X,Y,my_xor4)
f = @(x1, x2)(m4(ws,[x1,x2]));
[A,B] = meshgrid(0:0.1:1,0:0.1:1);
plot3d(f, A, B, true)
```

```
my_xor4(0,0)=0
my_xor4(0,1)=1
my_xor4(1,0)=1
my_xor4(1,1)=0

a =

     1
```



1.7 Comparison with Model 4 learned with Tensorflow

Weights of the hidden layer (manually copied):

[35]:
```
w11 = reshape([ 0.41652033,  0.7749157 ,  0.83778775,  0.64122725,  0.3972386 ,
         -0.13516521, -0.60432655, -0.20290181, -0.7232665 , -0.35317    ,
         -0.8889785 , -0.2863993 ,  0.54030126,  0.37175888, -0.82367843,
         -0.33497408, -0.8567182 ,  0.5161414 , -0.25462216,  0.59564906,
          0.80922335,  0.00252599,  0.3720131 , -0.1701207 ,  0.34805146,
         -0.38333094, -0.17244412,  0.7132528 , -0.14648864, -0.17876345].',␣
 ↪1,[]).';
w11 = [w11; [-0.6636416 ; -0.39717668]];
w12 = reshape([0.41662493, -0.7749062 , -0.8376726 , -0.64101034,  0.40976927,
         -0.09223783,  0.60428804, -0.09886253,  0.7417394 , -0.08979583,
          1.1194593 ,  0.13293397,  0.5400226 ,  0.37171456,  0.8246372 ,
         -0.43565178,  0.85677105,  0.51622313, -0.41895077, -0.5953253 ,
         -0.8091849 , -0.3766787 ,  0.28819063, -0.38122708,  0.34833792,
          0.15245543, -0.25060123, -0.7132655 , -0.30406952, -0.3443008].',␣
 ↪1,[]).';
w12 = [w12; [0.66343206; -0.03848529]];
```

```
b1 = reshape([-4.16518986e-01, -4.11640503e-05, -1.45169579e-05, -3.
↪96516771e-06,
        -1.09622735e-04,  0.00000000e+00,  2.90098578e-05,  0.00000000e+00,
        -1.63983065e-03,  0.00000000e+00, -6.36966957e-04, -1.47912502e-01,
        -5.39916575e-01, -3.71752203e-01, -5.50682598e-04,  1.15736163e+00,
        -6.27825721e-05, -5.16140461e-01,  0.00000000e+00, -1.62737619e-04,
        -8.02413124e-05, -2.25486048e-02,  1.79730232e-05,  0.00000000e+00,
        -3.48306417e-01, -1.66664287e-01,  0.00000000e+00, -3.03934885e-05,
         0.00000000e+00,  0.00000000e+00,  6.44910688e-05,  0.00000000e+00].',␣
↪1,[]).';
ws1=[w11,w12,b1];
ws1=reshape(ws1.',1,[]).';
```

Weights of the output layer manually copied:

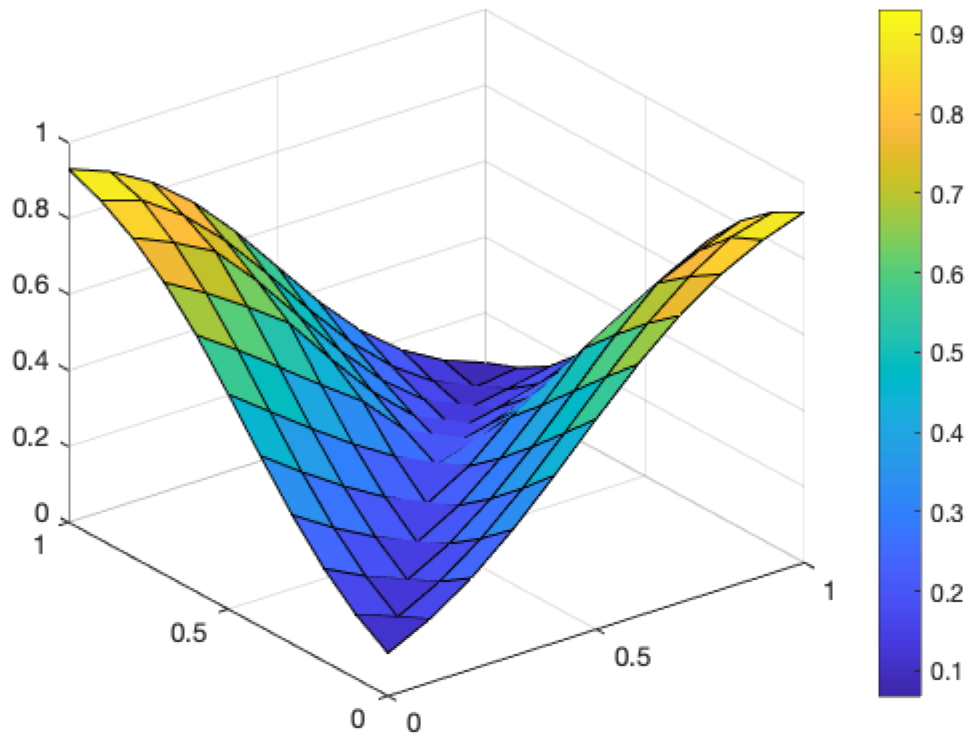
[36]:
```
ws2 = [-0.8178053 ,
1.0259871 ,
0.7672013 ,
0.9983522 ,
0.3300904 ,
0.1318875 ,
0.9221373 ,
0.20387506,
1.0057546 ,
0.2067241 ,
0.7479725 ,
-0.25578788,
-0.83140665,
-0.952559  ,
0.946334  ,
-1.0112743 ,
0.5946371 ,
-1.0230583 ,
-0.04098088,
0.9588608 ,
0.7448052 ,
-0.10435582,
0.25728533,
0.30141222,
-0.8235109 ,
-0.21171094,
-0.28320622,
1.0405817 ,
0.40911728,
0.37331975,
0.87603277,
```

```
0.19098908,
-0.8885394];
ws = [ws1;ws2];
```

Replace the learned weights of model m_4 with the copied weights and assess the function:

[37]:
```
my_xor5 = @(x1, x2)(round(m4(ws,[x1,x2])));
for i=1:4
    fprintf("my_xor5(%d,%d)=%d\n", X(i,1),X(i,2), my_xor5(X(i,1),X(i,2)))
end
a=accuracy(X,Y,my_xor5)
f = @(x1, x2)(m4(ws,[x1,x2]));
[A,B] = meshgrid(0:0.1:1,0:0.1:1);
plot3d(f, A, B, true)
```

```
my_xor5(0,0)=0
my_xor5(0,1)=1
my_xor5(1,0)=1
my_xor5(1,1)=0

a =

     1
```



1
0.8
0.6
0.4
0.2
0
1
0.5
0
0
0.5
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1