Numerical optimization for large scale problems and Stochastic Optimization

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Abstract

This report describes a possible approach to Problem 1, concerning *Static Optimization*. In particular, the proposed approach consists in building a Neural Network able to approximate a function, which values are accessible only through simulations. Then an optimization algorithm has been developed to obtain the argument that maximize the function, directly on the Neural Network.

1 Problem 1: Static Optimization

The Neural Network is composed by:

• Input layer: 2 input nodes (s1,s2) and 1 bias node

• Hidden layer: 2 hidden nodes and 1 bias node

• Output layer: 1 output node

As activation function has been used the sigmoid function:

$$h_{\theta}(x) = \frac{1}{1 + e^{-x}}$$

The learning rate used is $\mu = 0.01$ and at each step is multiplied by 0.9999. A *tolerance* of 10^{-6} has been used for the SSE error and the number of epochs is setted at 10000.

1.1 Commented code

The following scripts written in Python language have been used to solve the problem.

```
[1]: import numpy as np
  import pandas as pd
  import math
  import random
  import datetime
  import itertools
```

```
[2]: # function for probabilities
def compute_probabilities(s1, s2):

p12 = 1/60 + (1/200 - 1/60) * math.sqrt(1-((10-s1)/10)**2)
p23 = 1/30 + (1/100 - 1/30) * math.sqrt(1-((10-s2)/10)**3)
```

```
return p12, p23
```

```
[3]: # function for 60days scheduling
     def scheduling(p12, p23, s1, s2):
         #for the 1st day
         n12 = 2000
         B12 = np.random.binomial(n12, p12)
         W1 = B12
         B1 = 0
         N1 = 2000 - W1 - B1
         total_gain = 2000 - (s1+s2)
         last_gain = 0
         #all the other
         for i in range(1, 60):
             WO = W1
             B0 = B1
             n12 = 2000 - W0 - B0
             B12 = np.random.binomial(n12, p12)
             n23 = W0
             B23 = np.random.binomial(n23, p23)
             W1 = W0 + B12 - B23
             B1 = B23
             N1 = 2000 - W1 - B1
             daily_gain = (2000 - B1) * 1 - 90 * B1 - (s1+s2)
             total_gain = total_gain + daily_gain
             if i== 59:
                 last_gain = (2000 - B1) * 1 - 90 * B1
         return total_gain, last_gain
```

1.1.1 Simulation

```
[4]: now = datetime.datetime.now()
s_list = np.arange(2,11, 2)
combinations = list(itertools.product(s_list, s_list))
```

```
result = []
tot = []
# Start the simulation
for s1, s2 in combinations:
    p12, p23 = compute_probabilities(s1, s2)
   result.append(s1)
   result.append(s2)
   tot.append(s1)
   tot.append(s2)
   i_result = []
   tot_g = []
   for i in range(10000):
        tot_gain, last_gain = scheduling(p12, p23, s1, s2)
        i_result.append(last_gain)
        tot_g.append(tot_gain)
    result.append(i_result)
    tot.append(tot_g)
finish = datetime.datetime.now()
delta = finish - now
print(f"Start: {now}\nFinish: {finish}\nDeltaT:{delta}" )
```

Start: 2021-02-10 17:06:32.933865 Finish: 2021-02-10 17:07:53.521874 DeltaT:0:01:20.588009

1.1.2 Expected value for each pair (s1, s2)

```
[5]: expected_values = {}
    array = []

    final = []
    for r, (s1, s2) in zip(tot[2::3], combinations):
        expected_values[(s1,s2)] = sum(r)/10000
        array.append(sum(r)/10000)
```

```
[6]: values = np.array(array)
values
from scipy.stats import zscore
from sklearn import preprocessing

scaler = preprocessing.StandardScaler()
mean_training = values.mean()
```

```
std_training = values.std()
      max_training = max(values) # max values for normalization
      min_training = min(values) # min values for norm.
      # Max-min norm.
      normalized = [(x - min_training)/(max_training - min_training) for x in values]
      \#standardized = [(x - mean\_training)/(std\_training) for x in values]
      # Max-min Normalization for the output of the NN
      for (s1, s2) , st_value in zip(combinations, normalized):
          final.append([[s1,s2], [st_value]])
          print(f"Pair:{s1,s2} --> {st_value} ",)
     Pair:(2, 2) --> 0.0
     Pair:(2, 4) --> 0.3329668930670624
     Pair:(2, 6) --> 0.4894631578876288
     Pair:(2, 8) --> 0.543654801035603
     Pair: (2, 10) --> 0.5464052791490887
     Pair: (4, 2) --> 0.34731989670391716
     Pair: (4, 4) --> 0.6048384320283968
     Pair: (4, 6) --> 0.7277204108628127
     Pair:(4, 8) --> 0.767257188766194
     Pair: (4, 10) --> 0.7696519815083037
     Pair:(6, 2) --> 0.5596260220409397
     Pair: (6, 4) --> 0.7717083302275003
     Pair: (6, 6) --> 0.8732868634139147
     Pair:(6, 8) --> 0.90598264095888
     Pair:(6, 10) --> 0.9049712865254186
     Pair: (8, 2) --> 0.6752592855073805
     Pair:(8, 4) --> 0.8629338624781059
     Pair:(8, 6) --> 0.9523181734809203
     Pair:(8, 8) --> 0.9808865654175629
     Pair: (8, 10) --> 0.9795814229409096
     Pair:(10, 2) --> 0.710386103043338
     Pair:(10, 4) --> 0.888936206483296
     Pair: (10, 6) --> 0.9739154909636875
     Pair: (10, 8) --> 0.999878364208877
     Pair:(10, 10) --> 1.0
[22]: mean_training
[22]: 100981.20129999999
     1.1.3 Neaural Network
 [7]: # Normalization of the input
      X_{train} = np.zeros((25,2))
      for i, (s1, s2) in enumerate(combinations):
```

X_train[i,0] = s1/10
X_train[i,1] = s2/10

```
# output normalized
      y_train = normalized
 [8]: # activation function
      def sigmoid(x):
          return 1/(1+ np.exp(-x))
      def sigmoid_derivative(x):
          return x*(1-x)
 [9]: # function: convert normalized output to denormalized gain
      def convert_to_gain(x):
          return x*(max_training-min_training) + min_training
[10]: import numpy as np
      class NeuralNet():
          def __init__(self):
              np.random.seed(41)
              self.bias = np.random.rand(1) # o lo metto fisso ad 1?
              self.learning_rate = 0.2
          def update_weights(self, weights):
              self.weights = weights
          def sigmoid(self, x):
              return 1 / (1 + np.exp(-x))
          def sigmoid_der(self, x):
              return self.sigmoid(x)*(1-self.sigmoid(x))
          def training(self, X_train, output, tol):
              #
              bias = [1, 1, 1] # 2 for the 2 hidden neurons and 1 for the output
              weights = 0.5*np.random.rand(3, 3) # weights initialization
              #print(weights)
              # step lenght coefficient, mu
              coeff = 0.01
              #Initialization: SSE initialized at high value, flag: boolean for early stop_{\sqcup}
       → (reach tollerance), n_epochs
              sse\_old = 10000
              flag = False
              n_{epocs} = 10000
              for i in range(n_epocs):
```

```
if flag == True:
               print("Reached tol: ", tol)
               break
           out = np.zeros(25)
           numInput = X_train.shape[0] #len(X_train) #25 length of input
           for j in range(numInput):
               x2 = [0,0]
               # Feed forward
               # Hidden Layer
               # Hidden node 1
               H1 = bias[0]*weights[0,0] + X_train[j,0]*weights[0,1] + ____
\rightarrowX_train[j,1]*weights[0,2];
               x2[0] = sigmoid(H1);
               # Hidden node 2
               H2 = bias[1]*weights[1,0] + X_train[j,0]*weights[1,1] + _ \dots 
\rightarrowX_train[j,1]*weights[1,2];
               x2[1] = sigmoid(H2);
               # Output layer
               x3_1 = bias[2]*weights[2,0] + x2[0]*weights[2,1] + x2[1]*weights[2,2];
               out[j] = sigmoid(x3_1);
               # Backpropagation
               delta3_1 = out[j]*(1-out[j])*(output[j]-out[j]);
               # Propagate the delta backwards into hidden layers
               delta2_1 = x2[0]*(1-x2[0])*weights[2,1]*delta3_1;
               delta2_2 = x2[1]*(1-x2[1])*weights[2,2]*delta3_1;
               # Add weight changes to original weights
               # And use the new weights to repeat process.
               # delta weight = coeff*x*delta
               for k in range(3):# 1:3
                   if k == 0: # Bias cases
                       weights[0,k] = weights[0,k] + 2*coeff*bias[0]*delta2_1;
                       weights[1,k] = weights[1,k] + 2*coeff*bias[1]*delta2_2;
                       weights[2,k] = weights[2,k] + 2*coeff*bias[2]*delta3_1;
                   else: \#\% When k=2 or 3 input cases to neurons
                       weights[0,k] = weights[0,k] + 2*coeff*X_train[j,0]*delta2_1;
                       weights[1,k] = weights[1,k] + 2*coeff*X_train[j,0]*delta2_2;
```

```
weights[2,k] = weights[2,k] + 2*coeff*x2[k-1]*delta3_1;
            # methods: update weights
            self.update_weights(weights)
        # compute the SSE
        sse = (output-out)**2
        print("Error: ",sse.sum())
        # Early stop, reached tollerance
        if abs(sse.sum() -sse_old)< tol:</pre>
            print(f"Reached at epoch {i}: ",abs(sse.sum() -sse_old))
            flag = True
            break
        # update sse_old
        sse_old = sse.sum()
        # update coeff
        coeff = coeff*0.9999
    return out
# methods for prediction
def think(self, x_valid):
    bias = [1,1,1]
   weights = self.weights
   x2 = [0,0]
            # Hidden node 1
   H1 = bias[0]*weights[0,0]+ x_valid[0]*weights[0,1] + x_valid[1]*weights[0,2];
   x2[0] = sigmoid(H1);
            # Hidden node 2
   H2 = bias[1]*weights[1,0]+ x_valid[0]*weights[1,1] + x_valid[1]*weights[1,2];
   x2[1] = sigmoid(H2);
   x3_1 = bias[2]*weights[2,0] + x2[0]*weights[2,1] + x2[1]*weights[2,2];
   out = sigmoid(x3_1);
    return out
```

```
[11]: ## Training NN
net = NeuralNet()

tol = 10**(-6)
out= net.training(X_train, y_train, tol)
```

Error: 1.5644879423255782 Error: 1.5576685772752479 Error: 1.5514248395511812

Error: 0.19349412373873698 Error: 0.19349302940839494 Error: 0.1934919393631943 Error: 0.19349085359693105 Error: 0.19348977210341087 Error: 0.19348869487644724 Error: 0.19348762190986288 Error: 0.1934865531974897 Error: 0.19348548873316726 Error: 0.19348442851074535 Error: 0.19348337252408127 Error: 0.1934823207670417 Error: 0.19348127323350126 Error: 0.1934802299173446 Error: 0.19347919081246392 Error: 0.1934781559127608 Error: 0.19347712521214466 Error: 0.1934760987045349 Error: 0.19347507638385755 Error: 0.1934740582440495 Error: 0.19347304427905512 Error: 0.19347203448282715 Error: 0.1934710288493268 Error: 0.19347002737252555 Error: 0.19346903004640098 Reached at epoch 5998: 9.973261245743714e-07

1.1.4 Comparison

```
[12]: print("True - Predicted")
  tot_error = 0
  for i in range(len(out)):
      print(f"{y_train[i]:.4f} - {out[i]:.4f}, Error: {y_train[i] - out[i]}")
      tot_error += (y_train[i] - out[i])**2
print("SSE: ",tot_error)
```

```
True - Predicted
0.0000 - 0.2090, Error: -0.20902028020959426
0.3330 - 0.3172, Error: 0.015803499460750103
0.4895 - 0.4779, Error: 0.011553428883318617
0.5437 - 0.6527, Error: -0.10906014144621357
0.5464 - 0.7851, Error: -0.23870814356660597
0.3473 - 0.3322, Error: 0.015158083030664793
0.6048 - 0.4972, Error: 0.10767995919793438
0.7277 - 0.6698, Error: 0.05789414322410291
0.7673 - 0.7961, Error: -0.02889105805020975
0.7697 - 0.8688, Error: -0.09910371861850176
0.5596 - 0.5172, Error: 0.04247012374716641
0.7717 - 0.6866, Error: 0.08508326115273324
0.8733 - 0.8066, Error: 0.06671997953380426
0.9060 - 0.8744, Error: 0.031594375733392854
0.9050 - 0.9100, Error: -0.004992214684545138
```

```
0.6753 - 0.7029, Error: -0.02767100042908699

0.8629 - 0.8163, Error: 0.04664437249871456

0.9523 - 0.8795, Error: 0.07277696839614012

0.9809 - 0.9127, Error: 0.0682050595991267

0.9796 - 0.9303, Error: 0.04924477603949895

0.7104 - 0.8255, Error: -0.11508107321442052

0.8889 - 0.8843, Error: 0.004620425835072273

0.9739 - 0.9152, Error: 0.05874111403114113

0.9999 - 0.9317, Error: 0.06818579680965797

1.0000 - 0.9409, Error: 0.059082056805168426

SSE: 0.19346903004640092
```

1.1.5 Evaluate the result

```
[13]: # Start the evaluation
      now = datetime.datetime.now()
      result = []
      tot = []
      for s1, s2 in zip([2, 3, 1], [5, 9, 9]):
          p12, p23 = compute_probabilities(s1, s2)
          result.append(s1)
          result.append(s2)
          tot.append(s1)
          tot.append(s2)
          i_result = []
          tot_g = []
          for i in range(10000):
              tot_gain, last_gain = scheduling(p12, p23, s1, s2)
              i_result.append(last_gain)
              tot_g.append(tot_gain)
          result.append(i_result)
          tot.append(tot_g)
      finish = datetime.datetime.now()
      delta = finish - now
      print(f"Start: {now}\nFinish: {finish}\nDeltaT:{delta}" )
```

Start: 2021-02-10 17:07:57.607211 Finish: 2021-02-10 17:08:06.618197 DeltaT:0:00:09.010986

```
[21]: # compute the expected values
expected_values = {}
array = []

final = []
for r in (tot[2::3]):
```

```
#expected_values[(s1,s2)] = sum(r)/10000
array.append(sum(r)/10000)

## Print result
i = 0
for s1, s2 in zip([0.2, 0.3, 0.1], [0.5, 0.9, 0.9]):
    out= net.think([s1,s2])
    gain = convert_to_gain(out)

print(f"Expected gain from {s1}-{s2}: {array[i]:.2f} | Predicted: {gain:.2f}|_U
    →AbsolutError: {abs(array[i]- gain)} ")
    i = i+1
```

Expected gain from 0.2-0.5: 94921.77 | Predicted: 94195.57 | AbsolutError: 726.1974872872524 | Expected gain from 0.3-0.9: 99904.25 | Predicted: 102283.53 | AbsolutError: 2379.281943903261 | Expected gain from 0.1-0.9: 93874.53 | Predicted: 99301.67 | AbsolutError: 5427.143470283074

```
[15]: # Example of prediction: given an input it get the prediction normalized. Then

denormalized.
result = net.think([0.5,0.9])
print("Result normalized:", result)
print("Gain:",convert_to_gain(result))
```

Result normalized: 0.87173016070081

Gain: 103922.46083616714

1.1.6 Optimization

```
[16]: # Box projection: input constraints [0, 1]
  def box_projection(x):
    mins = [0,0]
    maxs = [1,1]
    xhat = np.maximum(np.minimum(x, maxs), mins);
    return xhat
```

```
[17]: # MU and C for Spall method
def mu(m):

    A = 10
    B = 100
    1 = 1
    return A/((B+m)**1)

def c(m):
    C=0.1
    t = 0.5
    return C/(m)**t

def spall_gradf(x, c):
    gradf = np.zeros(2)
```

```
h = (2*np.random.randint(0,2,size=(2))-1) # h: random vector -1, 1
          x_plus = x.copy() + c* h
          x_{minus} = x.copy() - c* h
          gradf = (net.think(x_minus.tolist()) - net.think(x_plus.tolist()))/(2*h)
          return gradf
[18]: # Armijo function
      def farmijo(fk, alpha, xk, pk, h):
          farm = fk - c1* alpha*np.dot(gradf(xk, h),pk)
          return farm
[19]: # Finite difference
      def gradf(x, h):
          gradf = np.zeros(2)
          # compute gradf
          for i in range(2):
              # centered finite difference
              x_plus = x.copy()
              x_{minus} = x.copy()
              x_plus[i]+= h
              x_minus[i]-=h
              \#gradf[i] = (net.think(x_plus.tolist()) - net.think(x_minus.tolist()))/(2*h)
              gradf[i] = (net.think(x_minus.tolist())- net.think(x_plus.tolist()))/(2*h)
          return gradf
[25]: x0 = np.random.rand(2) # random starting point between 0 and 1
      print("Starting point:", x0)
      print(f"Gain at x0: {convert_to_gain(net.think(x0))}")
      # Init
      h = 10**(-12)*np.linalg.norm(x0) # h value for finite difference
      gamma = 0.8 # factor that multiplies the descent direction before the (possible)
       → projection
      tolx = 10e-12 # a real scalar value characterizing the tolerance with respect to the
                     #norm of |xk+1 - xk| in order to stop the method;
      alpha0 = 0.7 #the initial factor that multiplies the descent direction at each
                   #iteration;
      c1 = 1e-4 # the factor of the Armijo condition that must be a scalar in (0,1);
      rho = 0.8 # fixed factor, lesser than 1, used for reducing alpha0;
      btmax = 50 # maximum number of steps for updating alpha during the backtracking
      tollgrad = 1e-12 #value used as stopping criterion w.r.t. the norm of the gradient;
      x = x0.copy()
      xk = box_projection(x) # projection
```

kmax = 10000 # max number of iterations

```
k = 0 # init k for iterations
fk = net.think(xk)
gradfk_norm = np.linalg.norm(gradf(xk, h))
deltaxk_norm = tolx +1
spall = False # set True: use Spall Method, False: finite difference
while k<kmax and gradfk_norm >= tollgrad and deltaxk_norm >= tolx:
    if spall == True:
        # gradient
        pk = -spall_gradf(xk, c(k+1))
        gamma = mu(k+1)
        #update x and step-length
        xbark = xk + gamma*pk
        # box proj. if exceed the constraint
        xhatk = box_projection(xbark)
        xnew = xhatk
        fnew = net.think(xnew)
        deltaxk_norm = np.linalg.norm(xnew - xk)
        xk = xnew
        fk = fnew
        gradfk_norm = np.linalg.norm(spall_gradf(xk, c(k+1)));
    else:
        # gradient
        pk = -gradf(xk, h)
        #update x and step-length
        xbark = xk + gamma*pk
        # box proj. if exceed the constraints
        xhatk = box_projection(xbark)
        # Reset the value of alpha for Armijo
        alpha = alpha0
        #compute the candidate xk
        pik = xhatk - xk
        xnew = xk + alpha*pik
        # compute the function f in xnew
        fnew = net.think(xnew)
        #Backtracing strategy with Armijo condition
        bt = 0
        while bt < btmax and fnew < farmijo(fk,alpha, xk, pik,h):
```

```
#Reduce the value of alpha
               alpha = rho * alpha
               # Update xnew and fnew w.r.t. the reduced alpha
               xnew = xk + alpha * pik
               fnew = net.think(xnew)
               # increase the counter
               bt = bt + 1
           # Update xk, fk, gradfk_norm, deltaxk_norm
           deltaxk_norm = np.linalg.norm(xnew - xk)
           xk = xnew
           fk = fnew
           gradfk_norm = np.linalg.norm(gradf(xk, h));
        # Increase the step by one
        k = k + 1;
    \rightarrow \{xk\}")
    if spall == True:
       print("Spall method")
        print("Finite difference")
    res = net.think(xk)
    print(f"Result:{fnew}")
    print(f"Optimized gain:{convert_to_gain(fnew)}")
   Starting point: [0.17768291 0.96347716]
   Gain at x0: 101473.22560120237
   -----
   End point at iteration K:30 ,xk:[1. 1.]
   Finite difference
   Result:0.9409237302420774
   Optimized gain:105326.29016417477
[]:
[]:
```

1.2 Neural Network results

The quality of the approximation has been evaluated at this three further values (s1 = 0.2; s2 = 0.5), (s1 = 0.3; s2 = 0.9), (s1 = 0.1; s2 = 0.9) and compared them with the prevision of the network. The following table provides the results obtained.

As might be expected the predicted result for [s1,s2] = [0.2, 0.5] has a relative low absolute error because

s1	s2	Simulation	Predicted	AbsError
0.2	0.5	94921.77	94195.57	726.197
0.3	0.9	99904.25	102283.53	2379.28
0.1	0.9	93874.53	99301.67	5427.14

the Neural Network has been trained with even numbers, so (s1=0.2) has already been seen. On the other hand, pair of odd numbers do not belong to the training set on which our model has been trained, so the approximations have higher absolute errors.

2 Optimization

This section explain a possible approach for the optimization task, which aim is to maximize the gain through the built model. In order to do that, we adapted the steepest descent method to work in this setting. However, since the function is not known in any explicit form, the gradient is not known and needs to be estimated from direct evaluations of the function f. Stochastic gradient method has been implemented with two approaches:

- Centered finite differences (CFD)
- Spall method

Spall method does simultaneous perturbation and requires only 2 function evaluations for each iteration, indeed the numerator is the same for each component, whereas the Centered FD requires 2*N function evaluation. In this problem, CFD works well since N=2 so there are no problem about the computational cost.

A box projection function has been implemented in order to maintain the constraint: $0 \le s1, s2 \le 10$.

2.1 Tuning parameter and Result

The initial point has been choosen randomly between 0 and 1 (since training inputs had been normalize with a decimal normalization). The explanation of the parameters is in section 1.1.6 Optimization at [25]. Obviously, precise values change at each trial, since there are variables (e.g. x0, h for Spall..) that are initialized as random.

2.1.1 Results: Spall

For the implementation of μ : A = 10, B = 100, l = 1 have been chosen. For the implementation of c : C = 0.1, t = 0.5 have been chosen.

tollgrad	tolx	х	Point	Gain	Iteration
10^{-12}	10^{-12}	x0:	[0.80272798 0.63937322]	104262	0
		xk:	[0.86038796 0.69303146]	104651	10000
10^{-12}	10^{-6}	x0:	[0.31179984 0.17112321]	91383	0
		xk:	[0.49885129 0.34086332]	97259	520
10^{-8}	10^{-6}	x0:	[0.23022621 0.77827517]	99672	0
		xk:	[0.35835989 0.89395774]	102831	288

As tolerances get smaller the number of iterations increases. In fact, as we can see in the first row of the table above the maximum number of iteration are reached. On the contrary the errors increase the number of iterations decreases, and an early stop criterion is reached. The expected maximum [1 1] is never reached, as a consequence the initial parameter μ and c can be tuned in order to get better results (with μ computed with: A = 1000, B = 500, l = 0.6 the maximum is reached after 25-50 iterations, depending on the starting point).

2.1.2 Results: Finite Difference

Case 1

For the implementation: γ : 0.8 as step-length, h: $10^{-6} * ||x||$ value for finite difference. For the Armijo's condition: α : 0.7, ρ : 0.8, btmax: 50 (max number of backtracking operations for Armijo).

tollgrad	tolx	Х	Point	Gain	Iteration
10^{-10}	10^{-10}	x0:	[0.04258496 0.76779936]	95810	0
		xk:	[1. 1.]	105326	26
10^{-8}	10^{-6}	x0:	[0.28295119 0.64437429]	98404	0
		xk:	[0.99999799 0.99999997]	105326	15

As ttolerances get smaller the number of iterations increases and the maximum [1 1] has been reached in the first row with just 26 iterations, whereas with a large tolerance an early stop occur after 15 iterations and it's very close to the optimum.

Case 2 : For the implementation: γ : 0.9 as step-length, h : $10^{-6} * ||x||$ value for finite difference. For the Armijo's condition: α : 0.75, ρ : 0.8, btmax: 50 (max number of backtracking operations for Armijo).

tollgrad	tolx	х	Point	Gain	Iteration
10^{-10}	10^{-10}	x0:	[0.70125869 0.13970315]	97685	0
		xk:	[1. 1.]	105326	19
10^{-8}	10^{-6}	x0:	[0.88571771 0.09344163]	100331	0
		xk:	[1. 0.99999897]	105326	15

In this case, both α and γ are increased. As a result, the function converge faster towards the optimum for both *tolerances* choice.

On the contrary, if α and γ are decreased the number of iterations increase.

Other tuning test could be done, even on the Armijo's parameter.

3 Plot

Here two plots of the points of the surfaces of the training set (left) and on the predicted data by the Network (right).



