Group MI1

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Machine Intelligence 1
WS 2020/21, Obermayer/Kashef

Exercise Sheet 3
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Multilayer Perceptrons and Backpropagation Algorithm

Exercise H3.1: Binary Classification (homework, 3 points)

For binary targets $y_T^{(\alpha)} \in \{0, 1\}$ the network output $y(\mathbf{x}; \mathbf{w}) \in (0, 1)$ can be interpreted as a probability $P(y = 1|\mathbf{x}; \mathbf{w})$. A suitable error function for this problem is:

$$E^T = \frac{1}{p}\sum_{\alpha=1}^{p} e^{(\alpha)}$$

with

$$e^{(\alpha)} = -\left[y_T^{(\alpha)} \ln y(\mathbf{x}^{(\alpha)}; \mathbf{w}) + (1 - y_T^{(\alpha)}) \ln\left(1 - y(\mathbf{x}^{(\alpha)}; \mathbf{w})\right)\right].$$

(a) (1 point) Show that

$$\frac{\partial e^{(\alpha)}}{\partial y(\mathbf{x}^{(\alpha)}; \mathbf{w})} = \frac{y(\mathbf{x}^{(\alpha)}; \mathbf{w}) - y_T^{(\alpha)}}{y(\mathbf{x}^{(\alpha)}; \mathbf{w})\left(1 - y(\mathbf{x}^{(\alpha)}; \mathbf{w})\right)}$$

(a) $\frac{\partial e^{(\alpha)}}{\partial y(\underline{x}^{(\alpha)}, \underline{w})} = -\frac{\partial}{\partial y(\underline{x}^{(\alpha)}, \underline{w})}\left[y_T^{(\alpha)} \ln y(\underline{x}^{(\alpha)}, \underline{w}) + (1-y_T^{(\alpha)}) \ln(1-y(\underline{x}^{(\alpha)}, \underline{w}))\right]$

$= -\frac{y_T^{(\alpha)}}{y(\underline{x}^{(\alpha)}, \underline{w})} - \frac{(1-y_T^{(\alpha)})\cdot(-1)}{1-y(\underline{x}^{(\alpha)}, \underline{w})}$

$= \frac{-y_T^{(\alpha)}(1-y(\underline{x}^{(\alpha)}, \underline{w})) + y(\underline{x}^{(\alpha)}, \underline{w})(1-y_T^{(\alpha)})}{y(\underline{x}^{(\alpha)}, \underline{w})(1-y(\underline{x}^{(\alpha)}, \underline{w}))}$

$= \frac{y(\underline{x}^{(\alpha)}, \underline{w}) - y_T^{(\alpha)}}{y(\underline{x}^{(\alpha)}, \underline{w})(1-y(\underline{x}^{(\alpha)}, \underline{w}))}$ □.

(b) (1 point) Consider an MLP with one hidden layer. The nonlinear transfer function for the output neuron ($i = 1, v = 2$) is assumed to be

$$f(h_1^2) = \frac{1}{1 + \exp(-h_1^2)},$$

where h_1^2 is the total input[1] of the output neuron. Show that its derivative can be expressed as

$$f'(h_1^2) = f(h_1^2)\left(1 - f(h_1^2)\right).$$

(b): $f(h_1^2) = \frac{1}{1+e^{-h_1^2}}$

$f'(h_1^2) = \frac{\partial}{\partial h_1^2}\left[\frac{1}{1+e^{-h_1^2}}\right] = \frac{-(-1)\cdot e^{-h_1^2}}{(1+e^{-h_1^2})^2} = \frac{(1+e^{-h_1^2})-1}{(1+e^{-h_1^2})^2}$

$= f(h_1^2) - f^2(h_1^2)$

$= f(h_1^2)[1 - f(h_1^2)]$ □.

(c) (1 point) Using the results from (a) and (b), show that the gradient of the error function $e^{(\alpha)}$ with respect to the weight w_{1j}^{21} between the the single output neuron ($i = 1, v = 2$) and neuron j of the hidden layer ($j > 0, v = 1$) is

$$\frac{\partial e^{(\alpha)}}{\partial w_{1j}^{21}} = \left(y(\mathbf{x}^{(\alpha)}; \mathbf{w}) - y_T^{(\alpha)}\right) f(h_j^1).$$

(c) $\frac{\partial e^{(\alpha)}}{\partial w_{1j}^{21}} = \frac{\partial e^{(\alpha)}}{\partial y(\underline{x}^{(\alpha)}, \underline{w})}\frac{\partial y(\underline{x}^{(\alpha)}, \underline{w})}{\partial w_{1j}^{21}}$

$\frac{\partial y(\underline{x}^{(\alpha)}, \underline{w})}{\partial w_{1j}^{21}} = \frac{\partial f(h_1^2)}{\partial h_1^2}\cdot\frac{\partial h_1^2}{\partial w_{1j}^{21}}$, where $\frac{\partial h_1^2}{\partial w_{1j}^{21}} = f(h_j^1)$

$= f'(h_1^2)$

> also, $y(\underline{x}^{(\alpha)}, \underline{w}) = f(h_1^2)$.

$\Rightarrow \frac{\partial e^{(\alpha)}}{\partial w_{1j}^{21}} = \frac{y(\underline{x}, \underline{w}) - y_T^{(\alpha)}}{y(\underline{x}^{(\alpha)}, \underline{w})(1-y(\underline{x}^{(\alpha)}, \underline{w}))}\cdot f(h_1^2)[1-f(h_1^2)]\, f(h_j^1)$

$\frac{\partial e^{(\alpha)}}{\partial w_{1j}^{21}} = \left[y(\underline{x}^{(\alpha)}, \underline{w}) - y_T^{(\alpha)}\right] f(h_j^1)$ □.

Exercise H3.2: MLP Regression (homework, 7 points)

The task is to implement an MLP with one hidden layer and apply the backpropagation algorithm to learn its parameters for a regression task.

Training Data: The file `RegressionData.txt` from the ISIS platform contains a small training dataset $\{x^{(\alpha)}, y_T^{(\alpha)}\}$, $\alpha = 1, \ldots, p$ with $p = 10$. The input values $\{x^{(\alpha)}\}$ in the first column are random numbers drawn from a uniform distribution over the interval $[0, 1]$. The target values $\{y_T^{(\alpha)}\}$ were generated using the function $\sin(2\pi x^{(\alpha)})$ and Gaussian noise with standard deviation $\sigma = 0.25$ was added [2].

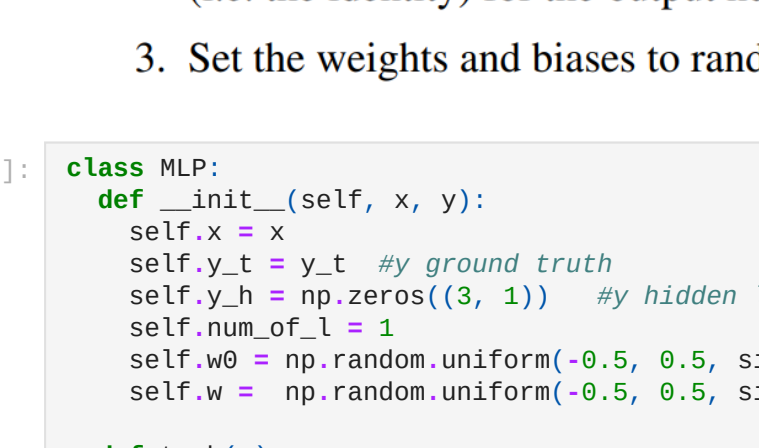
In [22]:
```
import numpy as np
import math
import matplotlib.pyplot as plt
```

In [23]:
```
from google.colab import drive
drive.mount('/content/drive')
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).
```

In [24]:
```
PATH_TO_DATA = '/content/drive/MyDrive/BCCN/Courses/Machine Intelligence/Machine Intelligence I/Exercise She
```

In [25]:
```
raw_data = np.genfromtxt(fname=PATH_TO_DATA, dtype=np.float)

x = raw_data[:,0]
y_t = raw_data[:,-1]

# Visualise Raw Data
plt.scatter(x,y_t)
plt.show()
```



(A) **Initialization:**

1. Construct the MLP using a single hidden layer with 3 hidden nodes ($N_1 = 3$) and an output layer with a single output neuron ($N_L = N_2 = 1$).
2. Use the tanh transfer function for the hidden neurons and the linear transfer function (i.e. the identity) for the output neuron.
3. Set the weights and biases to random values from the interval $[-0.5, 0.5]$.

In [26]:
```
class MLP:
  def __init__(self, x, y):
    self.x = x
    self.y_t = y_t  #y ground truth
    self.y_h = np.zeros((3, 1))   #y hidden layer
    self.num_of_l = 1
    self.w0 = np.random.uniform(-0.5, 0.5, size=(3,2))
    self.w =  np.random.uniform(-0.5, 0.5, size=(1,4))

  def tanh(x):
    return np.tanh(x)

  def dtanh(self, x):
    return 1 - np.tanh(x)**2
```

(B) **Iterative learning:**

1. For each input value $x^{(\alpha)}$ of the training set, do:
   (a) **Forward Propagation:** Calculate the total input and activity of the hidden neurons and the output neuron.
   (b) Compute the **output error** $e^{(\alpha)}$ using the quadratic error cost function.
   (c) **Backpropagation:** Calculate the "local errors" δ_i^v for the output and the hidden layer for each training point.
   (d) Calculate the gradient of the error function w.r.t. the first and second layer weights w_{ij}^{10} and w_{ij}^{21} respectively [3].
2. Calculate the batch gradient in order to obtain the direction of the weight updates:

$$\Delta w_{ij}^{v'v} = -\frac{\partial E^T_{[\mathbf{w}]}}{\partial w_{ij}^{v'v}} = -\frac{1}{p}\sum_{\alpha=1}^{p}\frac{\partial e^{(\alpha)}_{[\mathbf{w}]}}{\partial w_{ij}^{v'v}}$$

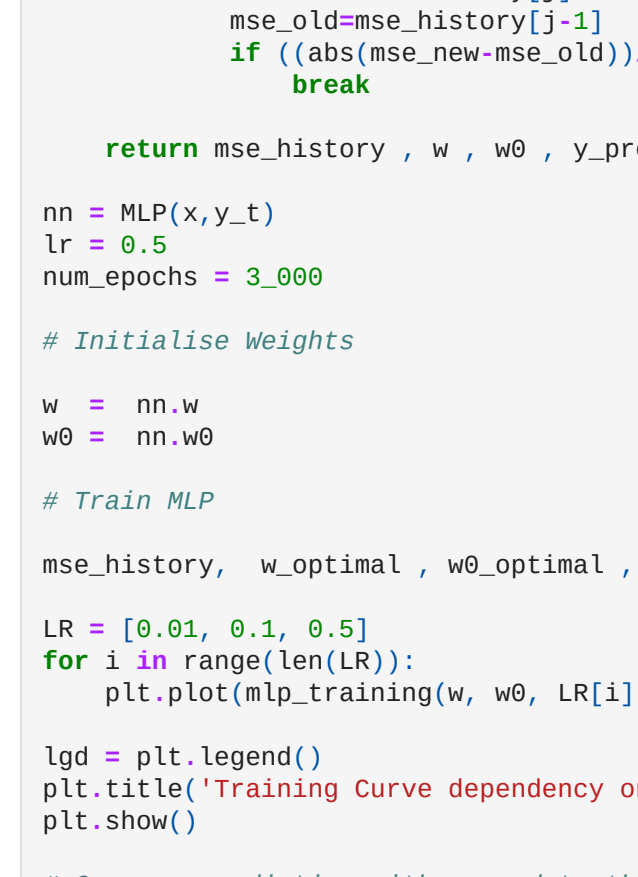
where $j = 0, \ldots, N_v$ and $i = 1, \ldots, N_{v'}$

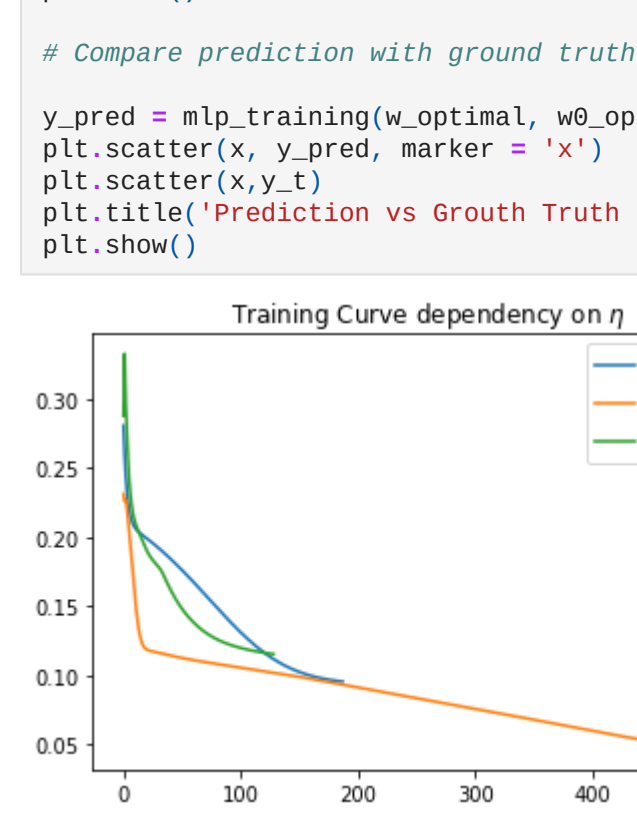
3. **Weight update:** Use gradient descent with a fixed learning rate $\eta = 0.5$ to update the weights in each iteration according to

$$\underline{\mathbf{w}}^{(t+1)} = \underline{\mathbf{w}}^{(t)} + \eta\Delta\underline{\mathbf{w}}^{(t)}$$

(C) **Stopping criterion:**
Stop the iterative weight updates if the error E^T has converged, i.e. $|\Delta E^T|/E^T$ has fallen below some small value (e.g. 10^{-5}) or a maximum number of iterations $t_{max} = 3000$ has been reached.

In [27]:
```
nn = MLP(x, y_t)
def mlp_training( w, w0 , lr = 0.5, num_epochs = 3_000, training = True):

    mse_history = []

    for j in range(num_epochs):

        mse = 0
        y_pred = []

        # For each of the training examples do:

        for i in range(len(x)):

            # Forward Pass

            # Pass input
            input = np.array([-1, x[i]])          # input with bias to hidden layer

            h1 = np.dot(w0, input.T)             # Net input pass to hidden layer
            z1 = np.tanh(h1)                     # Pass activation function


            z1 = np.hstack((-1, z1))              # Insert bias node

            h2 = np.dot(w,z1.T)
            y = h2                                # linear/identity activaion


            if not training:

                y_pred += [y]

            # Calculate error

            error       = 0.5*(y_t[i] - y)**2

            grad_error  = (y - y_t[i])


            if training :
                # Backward Pass

                del_L = 1
                del_hidden = nn.dtanh(h1).reshape(1,3)*w[:,1:]*del_L


                # Calculate Gradients
                grad_w   = (grad_error*del_L*z1).reshape(1,4)
                grad_w0  = (grad_error*del_hidden*(input.reshape(2,1))).T

                # Do the weight update

                w  = w  - lr*grad_w
                w0 = w0 - lr*grad_w0

            mse  += error

        # Append Epoch mean error
        mse_history += [mse/10]

        #stopping criterion
        if j>1:
            mse_new=mse_history[j]
            mse_old=mse_history[j-1]
            if ((abs(mse_new-mse_old))/mse_new)<=1e-3:
                break

    return mse_history , w , w0 , y_pred

nn = MLP(x,y_t)
lr = 0.5
num_epochs = 3_000

# Initialise Weights

w  = nn.w
w0 = nn.w0

# Train MLP

mse_history,  w_optimal , w0_optimal , y_pred = mlp_training(w, w0, 0.01)

LR = [0.01, 0.1, 0.5]
for i in range(len(LR)):
    plt.plot(mlp_training(w, w0, LR[i])[0], label = ' $\eta$ = %s' % LR[i]  )

lgd = plt.legend()
plt.title('Training Curve dependency on $\eta$')
plt.show()

# Compare prediction with ground truth data and we use the best learning rate we have.

y_pred = mlp_training(w_optimal, w0_optimal, 0.1, training = False)[-1]
plt.scatter(x, y_pred, marker = 'x')
plt.scatter(x,y_t)
plt.title('Prediction vs Grouth Truth upon Training')
plt.show()
```



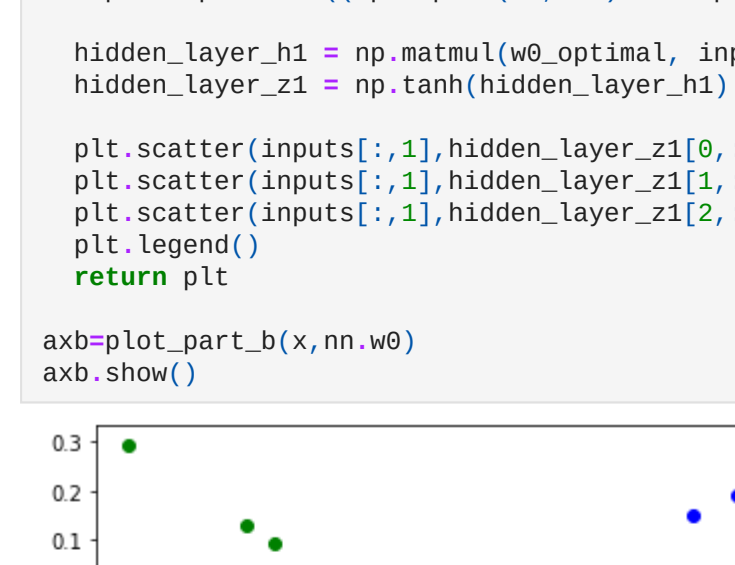


Note about learning rate dependency: A learning rate leads to a divergence after running for a large number of epochs such as 3000. So, conservatively, we choose for running for a large number of epochs.

Devliverables:

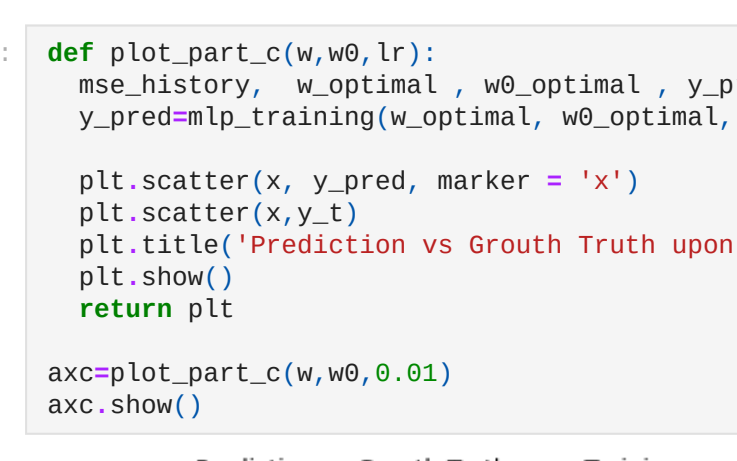
(a) (2 point) Plot the error E^T over the iterations.

In [28]:
```
def training_curve(w,w0,lr):
    mse_history= mlp_training(w, w0, lr)[0]
    f1, (ax1) = plt.subplots(1)
    ax1.plot(mse_history)
    ax1.set_xlabel('Epoch Number')
    ax1.set_ylabel('Mean Squared Error')
    ax1.set_title('MLP Training Curve')
    return ax1

axa=training_curve(nn.w,nn.w0,0.01)
```



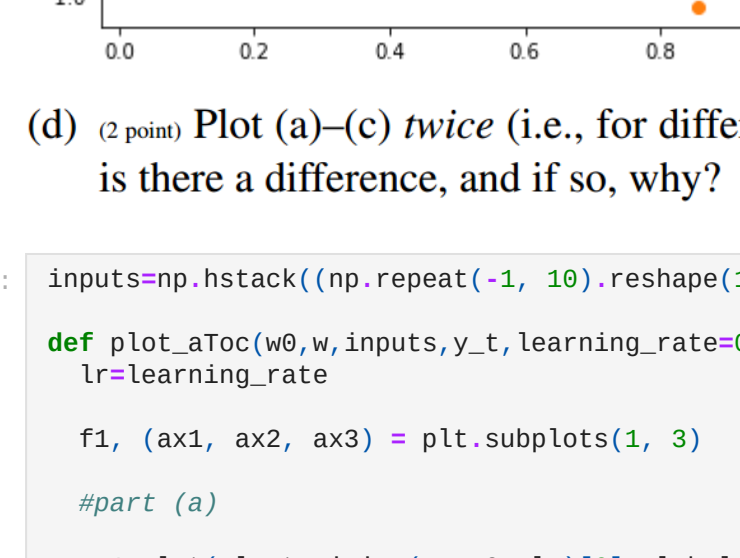
(b) (1 point) For the final network, plot the output of hidden units for all inputs.

In [29]:
```
# make a function out of it
def plot_part_b(x,w0):
    inputs=np.hstack((np.repeat(-1, 10).reshape(10,1) , x.reshape(10,1)))

    hidden_layer_h1 = np.matmul(w0_optimal, inputs.T)
    hidden_layer_z1 = np.tanh(hidden_layer_h1)

    plt.scatter(inputs[:,1],hidden_layer_z1[0,:],c='r', label='hidden_neuron_1')
    plt.scatter(inputs[:,1],hidden_layer_z1[1,:],c='b', label='hidden_neuron_2')
    plt.scatter(inputs[:,1],hidden_layer_z1[2,:],c='g', label='hidden_neuron_3')
    plt.legend()
    return plt

axb=plot_part_b(x,nn.w0)
axb.show()
```



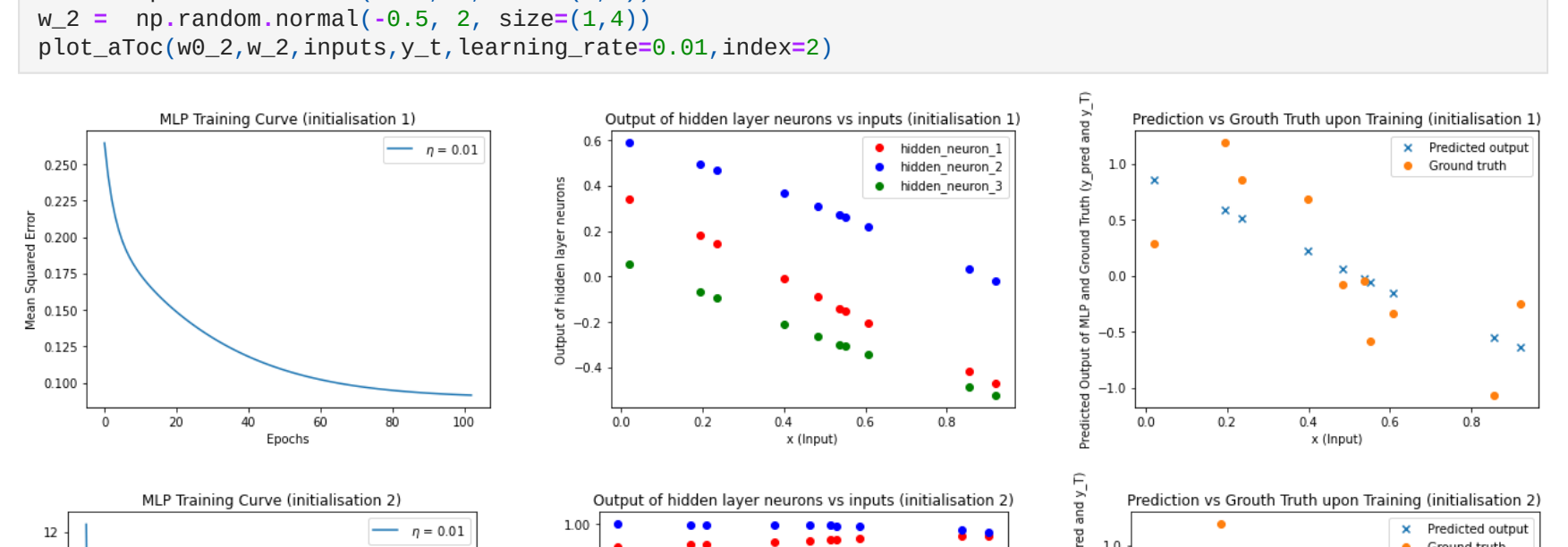
(c) (1 point) Plot the output values over the input space (i.e. the input-output function of the network) together with the training dataset.

In [30]:
```
def plot_part_c(w,w0,lr):
    mse_history,  w_optimal , w0_optimal , y_pred = mlp_training(w, w0, lr)
    y_pred=mlp_training(w_optimal, w0_optimal, lr, training = False)[-1]

    plt.scatter(x, y_pred, marker = 'x')
    plt.scatter(x,y_t)
    plt.title('Prediction vs Grouth Truth upon Training')
    plt.show()
    return plt

axc=plot_part_c(w,w0,0.01)
axc.show()
```



(d) (2 point) Plot (a)–(c) *twice* (i.e., for different initial conditions) next to each other and discuss: is there a difference, and if so, why?

In [32]:
```
inputs=np.hstack((np.repeat(-1, 10).reshape(10,1) , x.reshape(10,1)))

def plot_aToc(w,w0,inputs,y_t,learning_rate=0.01,index=1):
  lr=learning_rate

  f1, (ax1, ax2, ax3) = plt.subplots(1, 3)

  #part (a)

  ax1.plot(mlp_training(w, w0, lr)[0], label = ' $\eta$ = %s' % 0.01  )
  ax1.set_title('MLP Training Curve (initialisation %s)'% index)
  ax1.set_xlabel('Epochs')
  ax1.set_ylabel('Mean Squared Error')
  ax1.legend()

  #part(b)
  hidden_layer_h1 = np.matmul(w0, inputs.T)
  hidden_layer_z1 = np.tanh(hidden_layer_h1)

  ax2.scatter(inputs[:,1],hidden_layer_z1[0,:],c='r', label='hidden_neuron_1')
  ax2.scatter(inputs[:,1],hidden_layer_z1[1,:],c='b', label='hidden_neuron_2')
  ax2.scatter(inputs[:,1],hidden_layer_z1[2,:],c='g', label='hidden_neuron_3')

  ax2.set_title('Output of hidden layer neurons vs inputs (initialisation %s)'% index)
  ax2.set_xlabel('x (Input)')
  ax2.set_ylabel('Output of hidden layer neurons')
  ax2.legend()


  #part(c)
  mse_history,  w_optimal , w0_optimal , y_pred = mlp_training(w, w0, lr)
  y_pred=mlp_training(w_optimal, w0_optimal, lr, training = False)[-1]

  ax3.scatter(x, y_pred, marker = 'x',label='Predicted output')
  ax3.scatter(x,y_t,label='Ground truth')
  ax3.set_title('Prediction vs Grouth Truth upon Training (initialisation %s)'% index)
  ax3.set_xlabel('x (Input)')
  ax3.set_ylabel('Predicted Output of MLP and Ground Truth (y_pred and y_T)')
  ax3.legend()

  plt.subplots_adjust(left=0.2, bottom=0, right=3, top=1, wspace=0.3, hspace=5)
  plt.show()


np.random.seed(43)

#Initial condition 1
w0_1 = np.random.normal(-0.5, 0.5, size=(3,2))
w_1 =  np.random.normal(-0.5, 0.5, size=(1,4))
plot_aToc(w0_1,w_1,inputs,y_t,learning_rate=0.01,index=1)

#Initial condition 2
w0_2 = np.random.normal(-0.5, 2, size=(3,2))
w_2 =  np.random.normal(-0.5, 2, size=(1,4))
plot_aToc(w0_2,w_2,inputs,y_t,learning_rate=0.01,index=2)
```



In the first initialisation with smaller variance the mean squared error was smaller from the begining and slowly was lowering. The training of mlp with initialisation 2 (bigger variance) reduced cost function rapidly to a fraction and then lowered it slowly.

One could think, why the predictions are almost linear, do not reflect much the sinusoidal aspect of data. (It might be a bug) or it might be because the size of the network is much smaller than inputs and there are just two train points (first and last), that don't fit linearity well.

(e) (1 point) What might have been the motivation for using a quadratic error function here?

Using quadratic error function seems appropate, because the noise in the data is gaussian (by excersise design) and minimalising quadratic error function is the same as minimizing the variance of gaussian distributed data. Additionally, we know that optimal value exist and is unique.