Introduction to Neural Networks

Neural Networks

Neural Networks are a type of ML model

...Which follows a biology-inspired paradigm

- The idea is that the our brain achieves impressive results
- ...By relying on many (relatively simple) connected neurons

In fact, the first NNs were born as simplified biological models

Over time, the connection with biology has faded

Today, NNs are best understood as parameterized functions:

$$f(x, w)$$

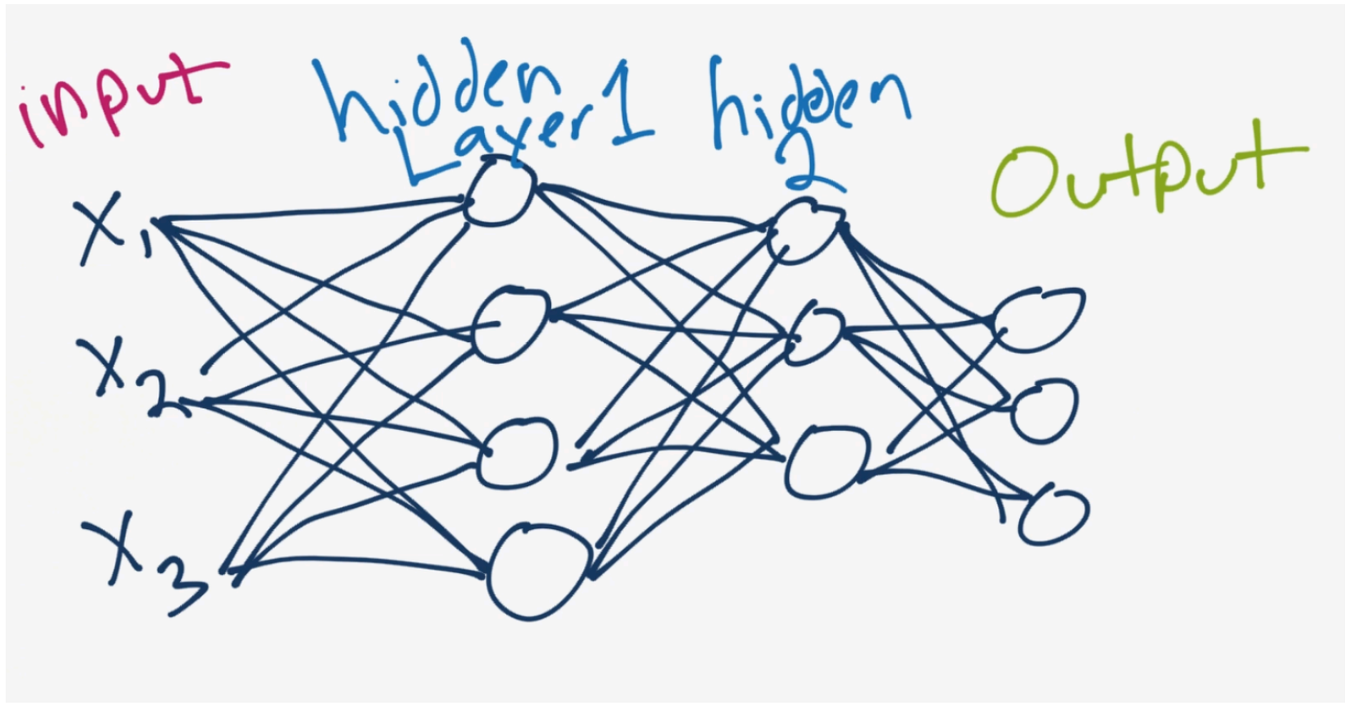
- Where x is the input vector
- ...And w is the parameter (weight) vector

The abstract definition is in fact close to that of Linear Regression

Neural Networks

The function f is made of multiple computation units called neurons

...That are connected via a variety of schemas



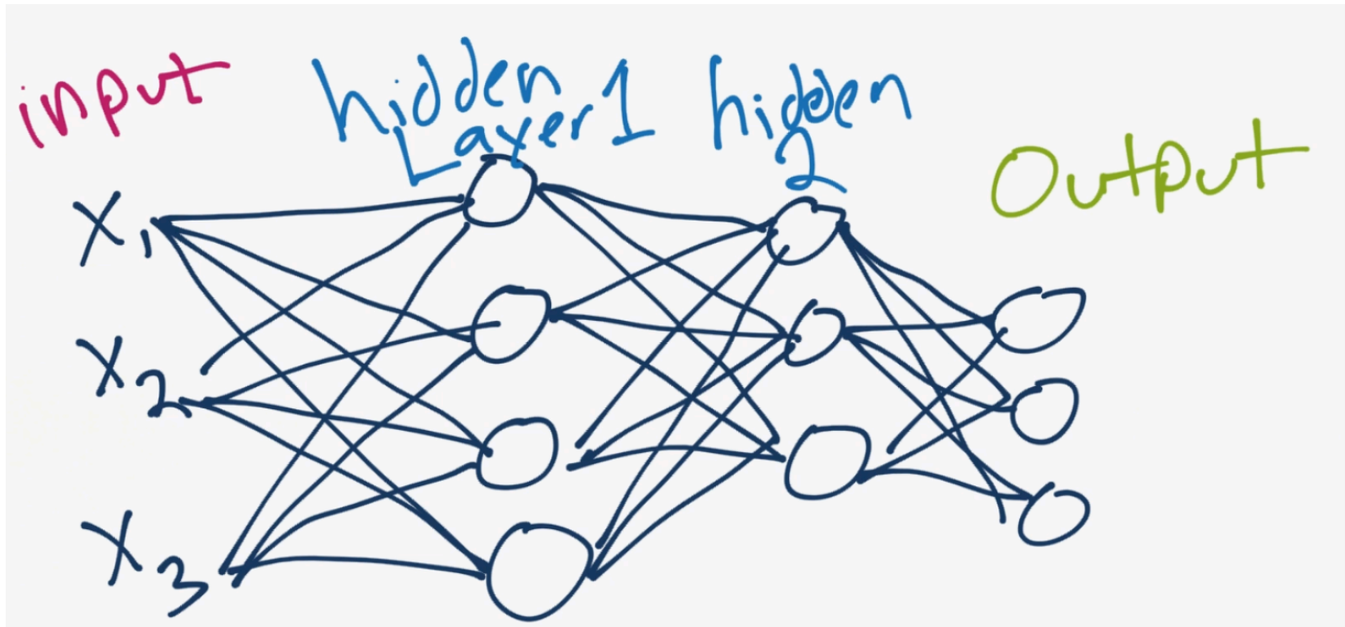
A popular schema (in the figure) consists in arranging neurons in layers

- Neurons in the same layer are not connected to each other
- Neurons in adjacent layers are fully connected

Neural Networks

The function f is made of multiple computation units called neurons

...That are connected via a variety of schemas

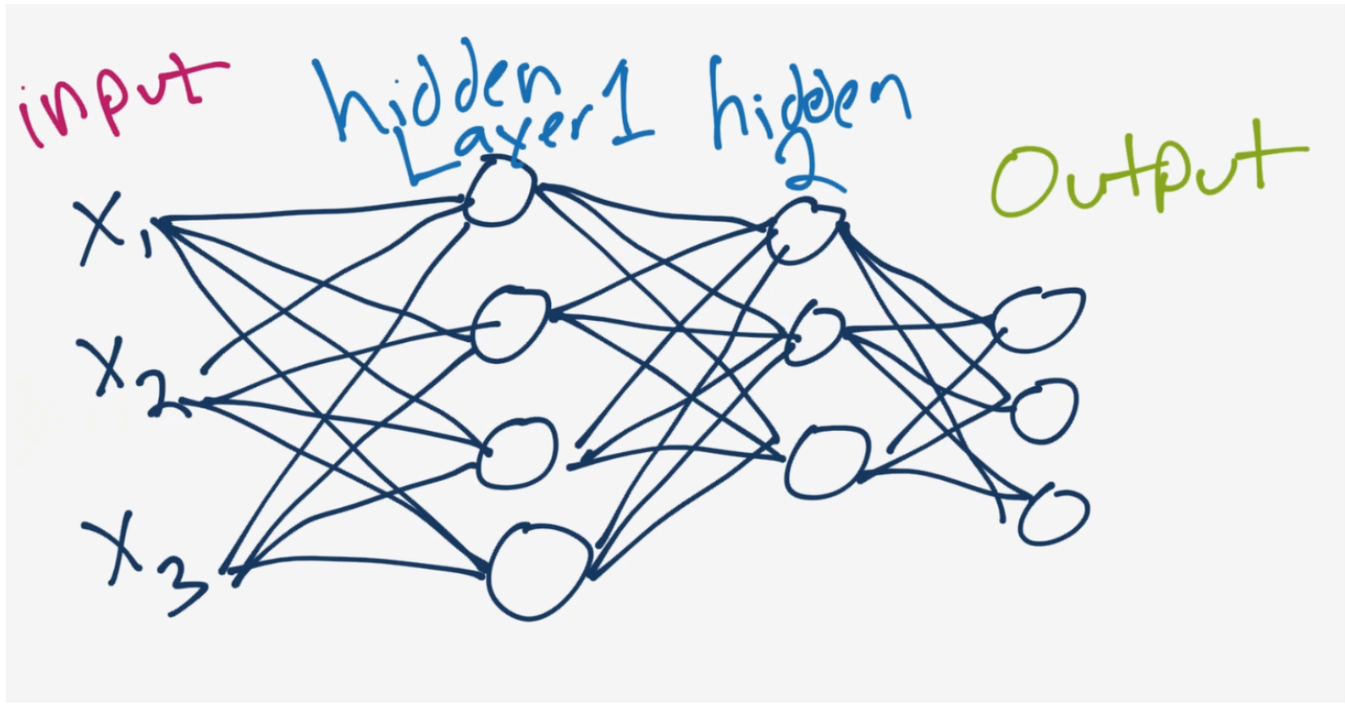


- The input is often treated as a first layer
- The final layer returns the output
- Intermediate layer are referred to as hidden

Neural Networks

The function f is made of multiple computation units called neurons

...That are connected via a variety of schemas



The resulting architecture is known as feed-forward, fully connected NN

- ...Or sometimes just as multilayer perceptron
- There are many more connection schemas
- ...But we will (mostly) stick to this one

Neurons

Each neuron is itself a (simple) parameterized function

In particular, most types of neurons have the form:

$$h(w^T x + \theta)$$

First the neuron computes $w^T x + \theta$

- This is just a weighted sum of its input (plus an offset)
- It's the same operation we do in Linear Regression

Then, the neuron applies an activation function h

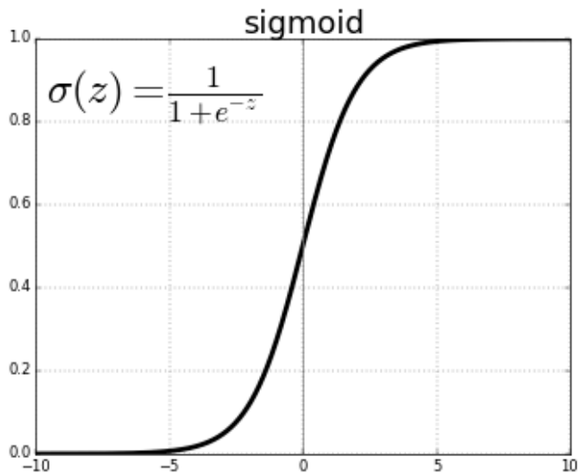
- This is univariate, scalar fuction (i.e. $h : \mathbb{R} \to \mathbb{R}$)
- ...And it's always monotone non-decreasing

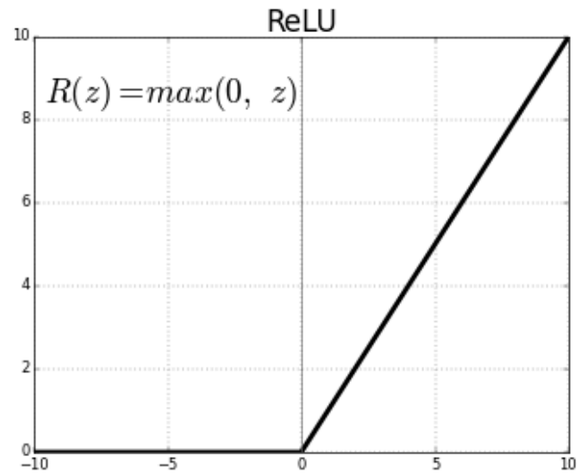
Using a linear activation function (i.e. $h(y) = y$) is a viable option

Neurons

However, activation functions are typically non-linear

Notable examples include





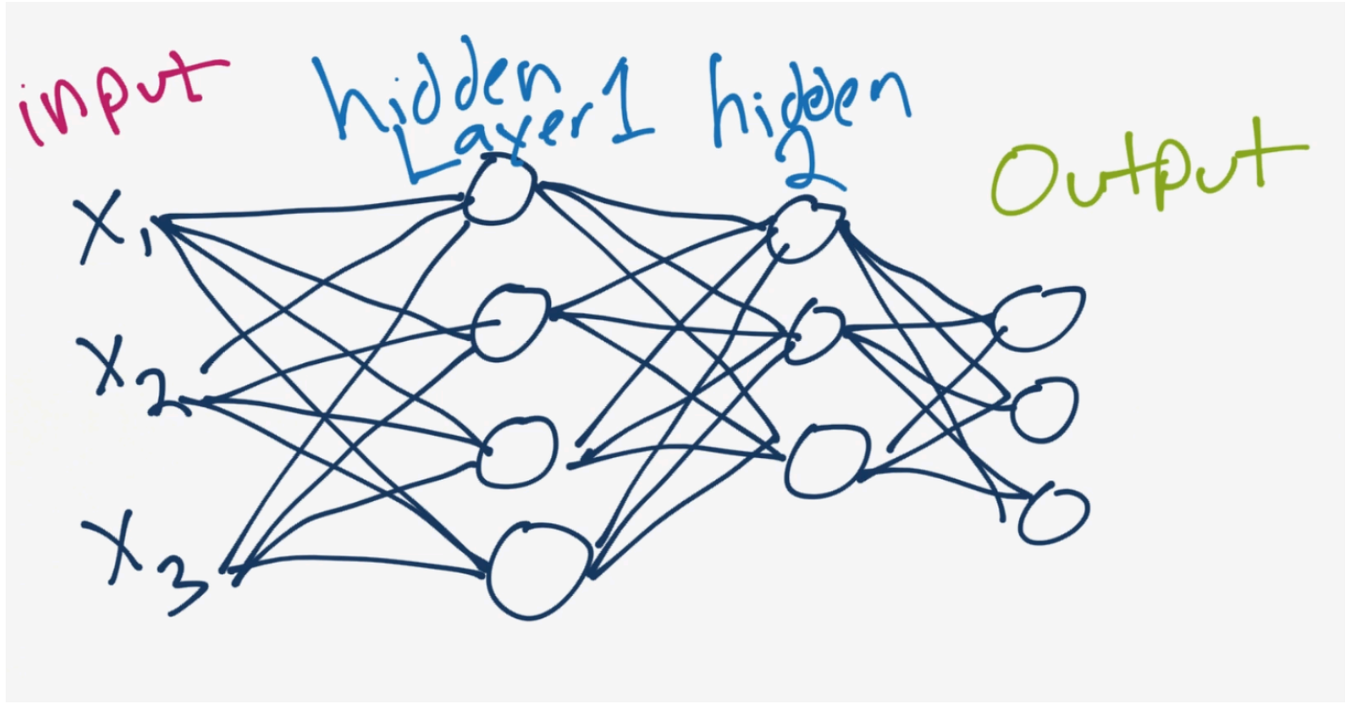
- A sigmoid is an example of a bounded activation function (in $[0, 1]$)
- A Rectifier Linear Unit is a piecewise linear activation function

Both provide a numerical characterization of the neuron state:

- If $w^T x + \theta \leq 0$, the neuron is inactive (the output is 0 or close)
- If $w^T x + \theta > 0$, the neuron is active (the output is positive)

NNs and Activation Functions

The properties of a MLP depend on the activation functions and layers

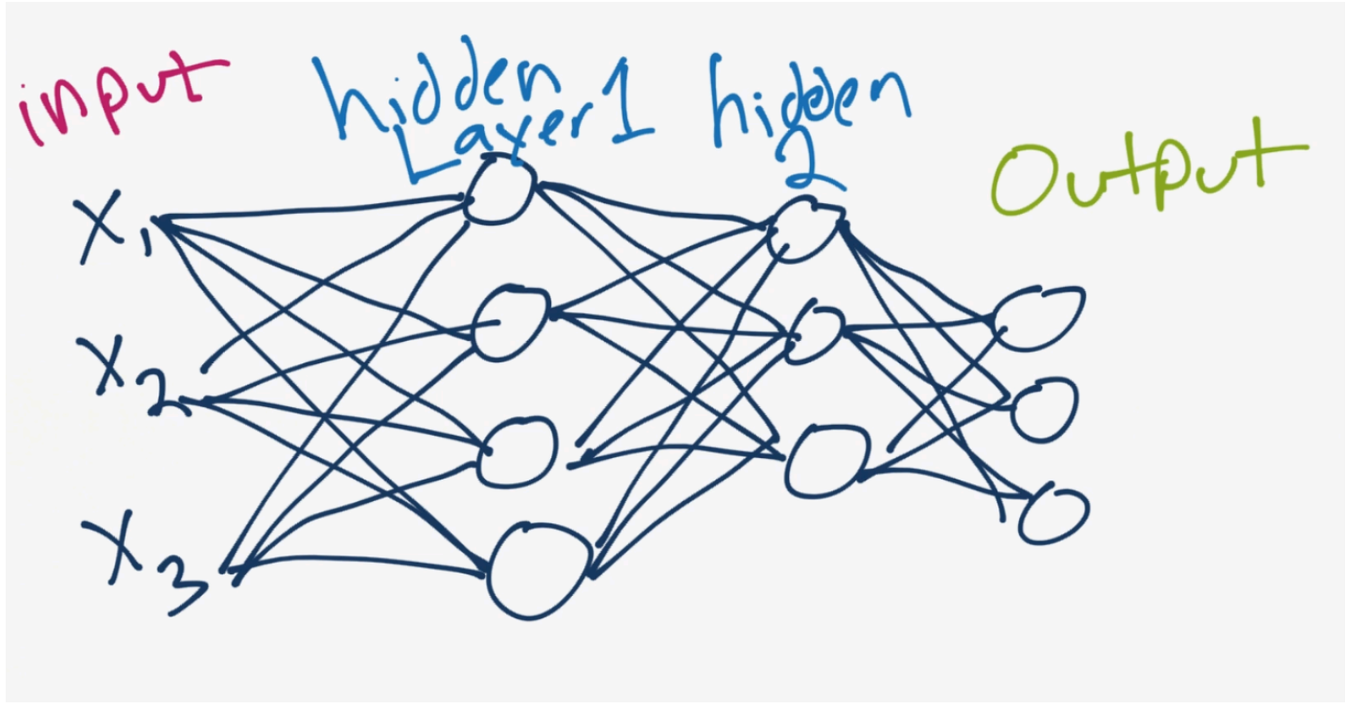


Let's start by discussing the activation function for the output layer:

- For regression tasks we typically choose a linear activation function
- ...Since that leaves the largest possible variability range for the output

NNs and Activation Functions

The properties of a MLP depend on the activation functions and layers

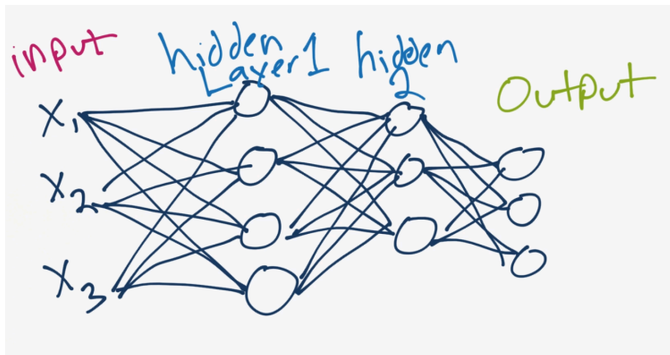


Let's start by discussing the activation function for the output layer:

- For classification tasks we typically choose a sigmoid (logistic function)
- ...Since that allow us to interpret outputs as probability values

NNs and Activation Functions

The properties of a MLP depend on the activation functions and layers



For classification tasks with multiple classes

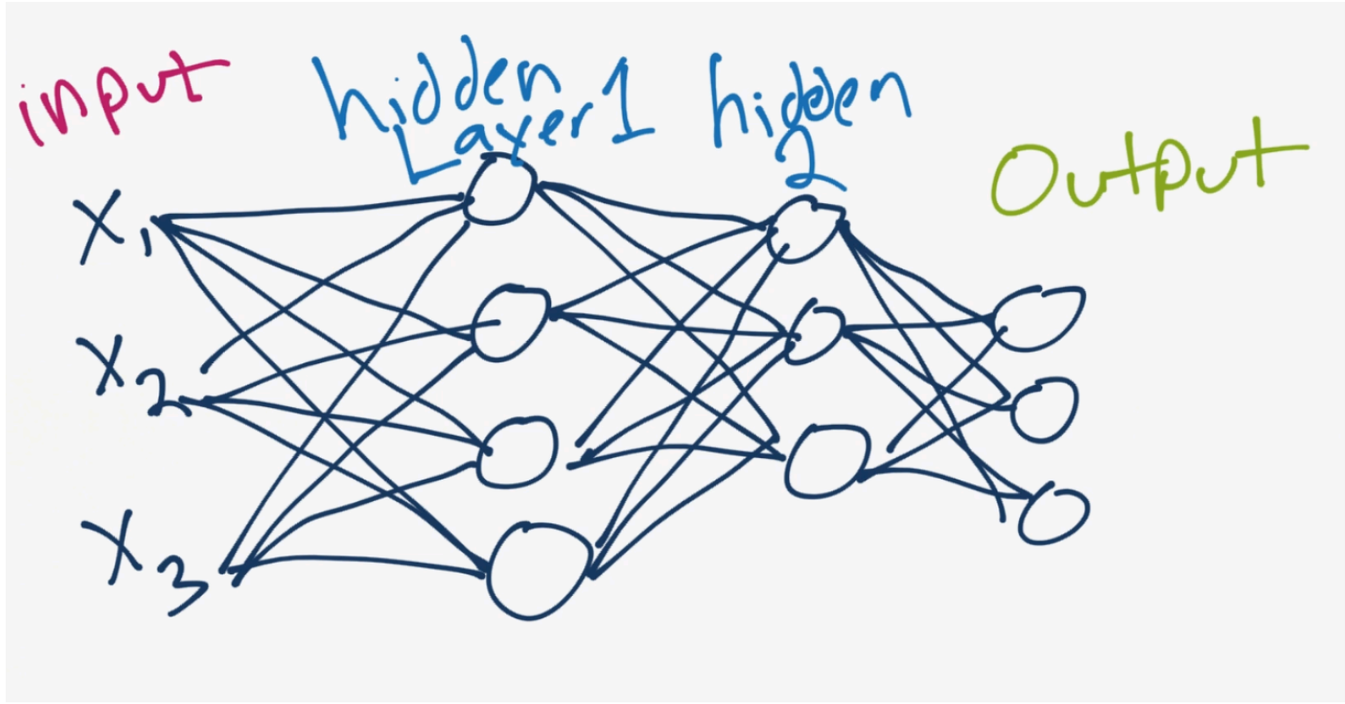
- We use one output neuron per class, with a sigmoid output
- ...Then we normalize the output so that they sum up to one
- This operation is called a softmax

Formally, this is defined as:

$$y_k(z) = \frac{e^{z_k}}{\sum_{k=1}^{n_k} e^{x_k}}$$

NNs and Activation Functions

The properties of a MLP depend on the activation functions and layers

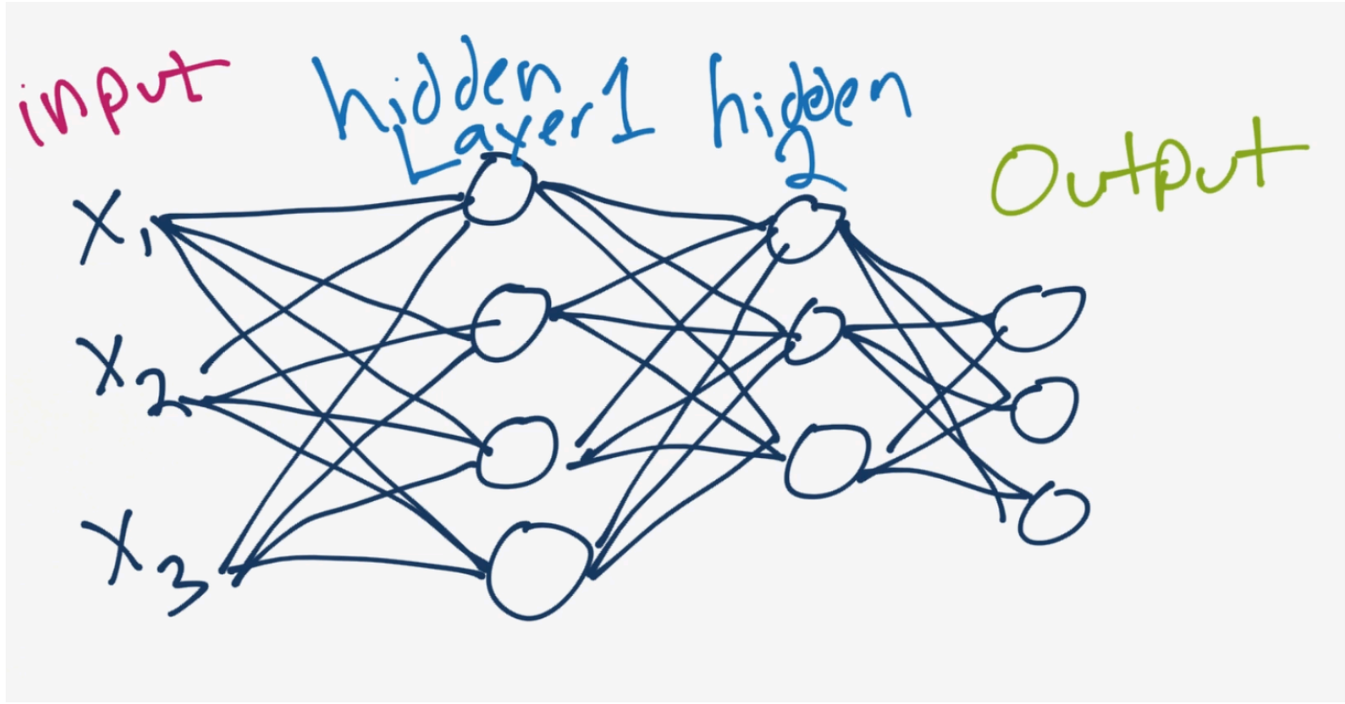


A MLP with no hidden layer is just a linear model!

- For regression, we get Linear Regression
- For classification, we get Logistic Regression
- ...The softmax "trick" is in fact borrowed from Logistic Regression

NNs and Activation Functions

The properties of a MLP depend on the activation functions and layers



For the hidden layers, we always use (at least some) non-linear functions

- In fact, if we used only linear activation functions
- ...We would get a linear model again

Universal Approximation

There is an important result about hidden layers and activation functions

- If a NN is sufficiently large
- ...And has at least one hidden layer
- ...With a non-linear activation function

Then the network can approximate any function with arbitrary precision

In other words, NNs are universal approximators

This is a very powerful result!

- No matter what input-output relation we need to learn
- ...With a large-enough NN and we have a good chance of succeeding

Just how big does the network need to be?

- It depends on the complexity of the true function to be learned
- ...And on the structure of the network

Shallow vs Deep NN

In particular, it depends on the number layers

Assuming that the ground truth function is challenging:

- If we use a single hidden layer, then that layer may need to be very large
- ...But if we use many hidden layers, they can be much smaller

We say that:

- A network is shallow if it has a single layer
- A network is deep if if has multiple layers

Deep learning is just NNs with multiple hidden layers

- In this lecture we will focus on shallow networks
- We will discuss deep networks in the next lecture

A Practical Example

We will try to learn an NN for our housing dataset

Let's start by loading the data

In [2]:
```
fname = os.path.join('data', 'real_estate.csv')
data = pd.read_csv(fname, sep=',')
in_cols = [c for c in data.columns if c != 'price per area']
X = data[in_cols]
y = np.log(data[['price per area']])
X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.34, random_state=42)

data.head()
```

Out[2]:

	house age	dist to MRT	#stores	latitude	longitude	price per area
0	14.8	393.2606	6	24.96172	121.53812	7.6
1	17.4	6488.0210	1	24.95719	121.47353	11.2
2	16.0	4066.5870	0	24.94297	121.50342	11.6
3	30.9	6396.2830	1	24.94375	121.47883	12.2
4	16.5	4082.0150	0	24.94155	121.50381	12.8

- Again, the first 4 colums are our input
- ...And our goal is to estimate $\log(\text{price per area})$

Building a Network in keras/tensorflow

We will rely on tensorflow and keras to deal with Neural Networks

- Tensorflow is a library for tensor computations developed by Google
- ...And Keras is a Python package to build and train NNs

For some years, Keras has been integrated in tensorflow

When working with NNs, our model does not have a fixed structure

...Instead, we need to decide how we want to build our NN

- Keras provides multiple approaches for constructing a NN model
- The simplest one is the so-called Sequential API
- ...Which requires to start by building a `Sequential` object

In [3]:
```
from tensorflow import keras

nn = keras.Sequential()
```


Building a Network in keras/tensorflow

Then we build a number of "layer" objects

...And we add then to the model

In [4]:
```
from keras.layers import Dense, Input

input_shape = (len(in_cols),)
nn.add(Input(input_shape))
nn.add(Dense(16, activation='relu'))
nn.add(Dense(1, activation='linear'))
```

- The first layer we add will be the one accepting the input
  - ...And for this reason we specify the size of the expected input vector
- The last layer we add will be the one providing the output

We have just built a shallow network

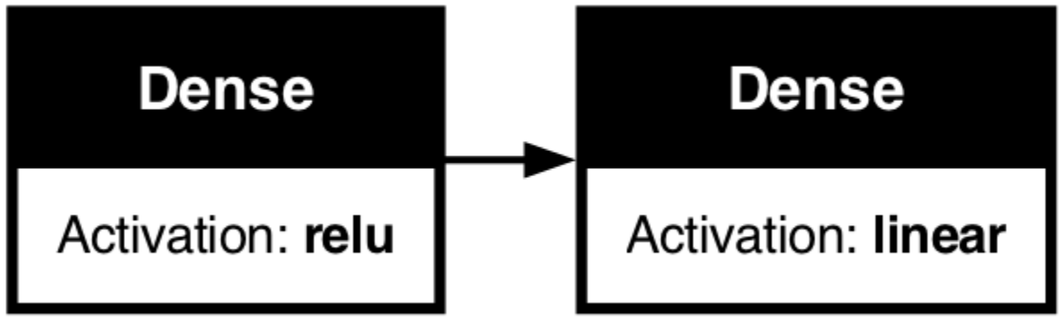
- The hidden layer has 16 neurons and a "ReLU" activation function
- The output layer contains a single, linear, neuron

Plotting a Model

We can even plot the model structure

In [5]:
```
keras.utils.plot_model(nn, rankdir='LR', show_layer_activations=True, dpi=150)
```

Out[5]:



- Every box represents a layer
- The first one is the input (which was added automatically by keras)
- The second is the ReLU layer that we explicitly added
- The last is the ouput layer

Note: you'll need to download the graphviz tool for this

Training a Neural Network

In principle, training a NN is the same as training a linear model

I.e. given a loss function $L(\hat{y}, f(\hat{x}, w))$ we need to solve:

$$\arg\min_{w} L(\hat{y}, f(\hat{x}, w))$$

- Where $\hat{x}$ is the training set input

For example, for an MSE loss we get:

$$\arg\min_{w} \|f(\hat{x}, w) - \hat{y}\|_2^2$$

- I.e. we want to tune the parmaters w
- ...So that our predictions $f(\hat{x}, y)$ are close to the targets $\hat{y}$

The main difference is that our function f is now non-linear

Training a Neural Network

For this reason, NNs are usually trained via gradient descent:

Starting from a parameter vector w_0, we repeat:

$$w_{k+1} = w_k - \eta_k \nabla_w L(\hat{y}, f(\hat{x}, w_k))$$

- I.e. we adjust the current parameter vector w_k
- ...In the direction opposite to the loss gradient $\nabla_w L(\hat{y}, f(\hat{x}, w_k))$

By doing this, we (roughly) cause the loss function to decrease

There are several algorithms based on gradient descent

E.g. Gradient Descent, Adagrad, AdadeIta, RMS Prop, Adam...

- They handle differently the step size η_k
- ...And sometimes they change other aspects of the process

Training a Neural Network

There is one specific "trick" that all approaches rely on

Rather than using all examples to compute the gradient:

$$w_{k+1} = w_k - \eta_k \nabla_w L(\hat{y}, f(\hat{x}, w_k))$$

...They instead randomly sample a subset $(\hat{x}', \hat{y}') \sim (\hat{x}, \hat{y})$:

$$w_{k+1} = w_k - \eta_k \nabla_w L(\hat{y}', f(\hat{x}', w_k))$$

This approach is known as Stochastic Gradient Descent

- Typically examples are first shuffled
- Then partitioned in small groups called mini-batches
- Then we run an gradient descent iteration over each mini-batch

Once all examples have been considered, we have completed an epoch

Standardizing the Data

Since we are using gradient descent

...It's in general a good idea to normalize/standardiza the data

- Gradient descent methods are affected by their startin point (i.e. $\boldsymbol{w}_0$)
- NN training libraries are very good at choosing those
- ...Provided that all inputs and output are reasonably close to 0

In [6]:
```
x_scaler, y_scaler = StandardScaler(), StandardScaler()
X_tr_s = x_scaler.fit_transform(X_tr)
X_ts_s = x_scaler.transform(X_ts)
y_tr_s = y_scaler.fit_transform(y_tr)
y_ts_s = y_scaler.transform(y_ts)
```

Skipping this step can makes training ineffective and/or unrealiable

Training a Neural Network in Keras

Training a Neural Network in Keras requires two steps

- First, se setup the training problem by calling the `compile` method
- Then, we start training by calling the `fit` method

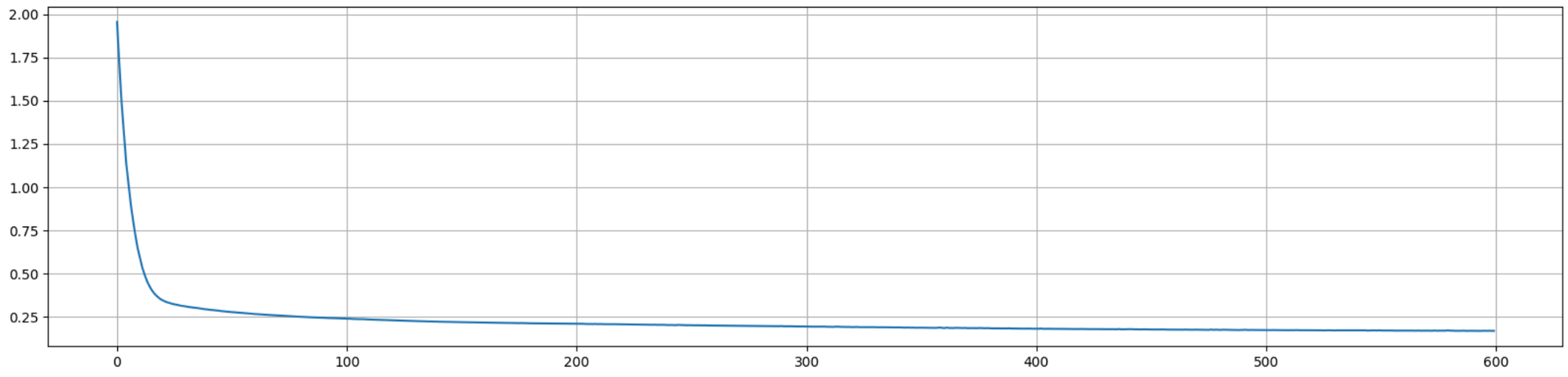
In [7]:
```
nn.compile(optimizer='adam', loss='mse')
history = nn.fit(X_tr_s, y_tr_s, batch_size=32, epochs=600)
```

```
Epoch 1/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 1.9172
Epoch 2/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 1.7323
Epoch 3/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 1.4560
Epoch 4/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 1.4367
Epoch 5/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 1.0571
Epoch 6/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 1.0502
Epoch 7/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 0.9954
Epoch 8/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 0.8611
Epoch 9/600
9/9 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 0.6867
```

Training a Neural Network in Keras

Let's plot the loss behavior over the epochs

In [8]:
```
loss_history = pd.Series(name='loss', data=history.history['loss'])
loss_history.plot(figsize=figsize, grid=':');
```



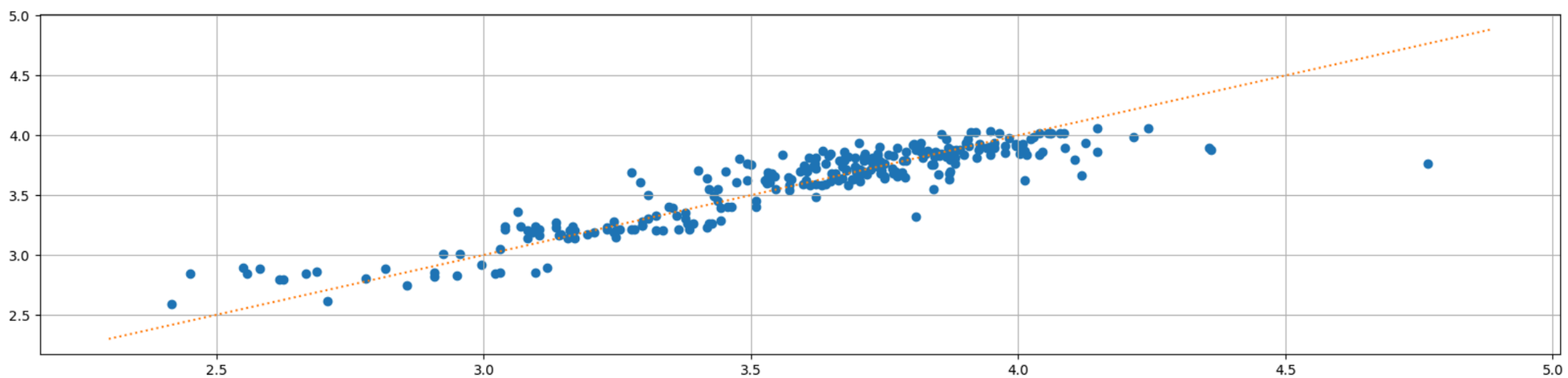
The flat behavior towards the end is due to the algorithm approaching convergence

Model Evaluation

NNs can be evaluated like any other ML model

Here are the results on the training set

In [9]:
```
nn_pred_tr = y_scaler.inverse_transform(nn.predict(X_tr_s, verbose=0))
plt.figure(figsize=figsize)
plt.scatter(x=y_tr, y=nn_pred_tr)
l, u = min(plt.xlim()[0], plt.ylim()[0]), max(plt.xlim()[1], plt.ylim()[1])
plt.plot([l, u], [l, u], linestyle=':', color='tab:orange')
plt.grid(); plt.show()
print(f'r2 score: {r2_score(y_tr, nn_pred_tr):.3f}')
```



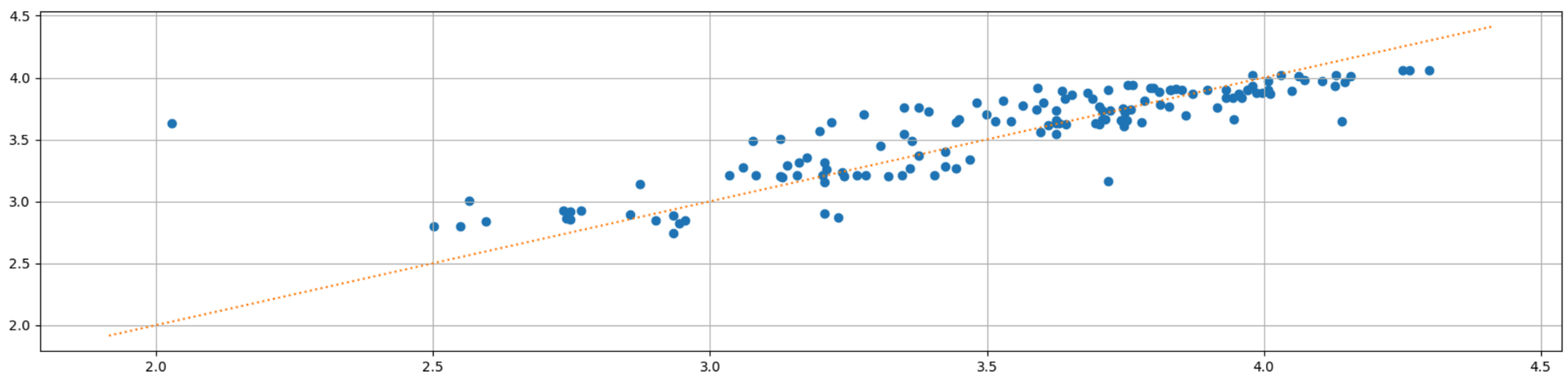
r2 score: 0.833

Model Evaluation

NNs can be evaluated like any other ML model

...And those on the test set

In [10]:
```
nn_pred_ts = y_scaler.inverse_transform(nn.predict(X_ts_s, verbose=0))
plt.figure(figsize=figsize)
plt.scatter(x=y_ts, y=nn_pred_ts)
l, u = min(plt.xlim()[0], plt.ylim()[0]), max(plt.xlim()[1], plt.ylim()[1])
plt.plot([l, u], [l, u], linestyle=':', color='tab:orange')
plt.grid(); plt.show()
print(f'r2 score: {r2_score(y_ts, nn_pred_ts):.3f}')
```



r2 score: 0.716

NN Output Surface

It's interesting to see how the NN output changes depending on the input

On this purpose, let's build a special dataset

- We will take one example as a reference
- Then build similar example by chaning a value of a single attribute

In [11]:
```
x_ref, a_ref = X_tr.iloc[120], 'dist to MRT'
a_vals = np.linspace(X_tr[a_ref].min(), X_tr[a_ref].max(), 1000)

x_sensitivity = pd.DataFrame(index=np.arange(len(a_vals)), columns=X_tr.columns)
for c in X_tr.columns:
    if c == a_ref: x_sensitivity[c] = a_vals
    else: x_sensitivity[c] = x_ref[c]
x_sensitivity.head()
```

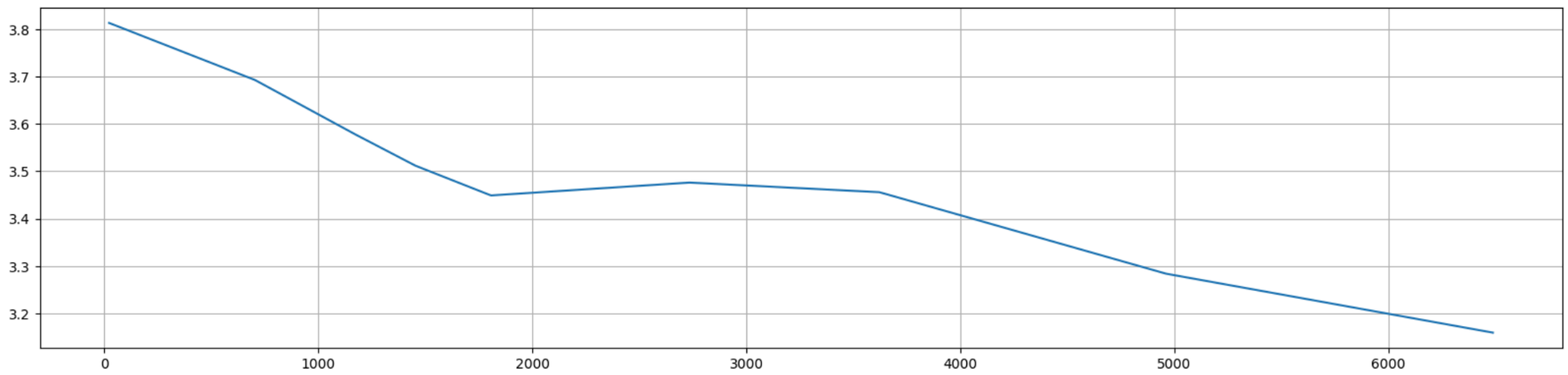
Out[11]:

	house age	dist to MRT	#stores	latitude	longitude
0	41.3	23.382840	6.0	24.96674	121.54039
1	41.3	29.853949	6.0	24.96674	121.54039
2	41.3	36.325059	6.0	24.96674	121.54039
3	41.3	42.796168	6.0	24.96674	121.54039
4	41.3	49.267277	6.0	24.96674	121.54039

NN Output Surface

Now, let's see how our NN response to changes in the attribute

In [12]:
```
nn_pred_s = y_scaler.inverse_transform(nn.predict(x_scaler.transform(x_sensitivity), verbose
pred_sensitivity = pd.Series(index=a_vals, data=nn_pred_s.ravel())
pred_sensitivity.plot(figsize=figsize, grid=':');
```

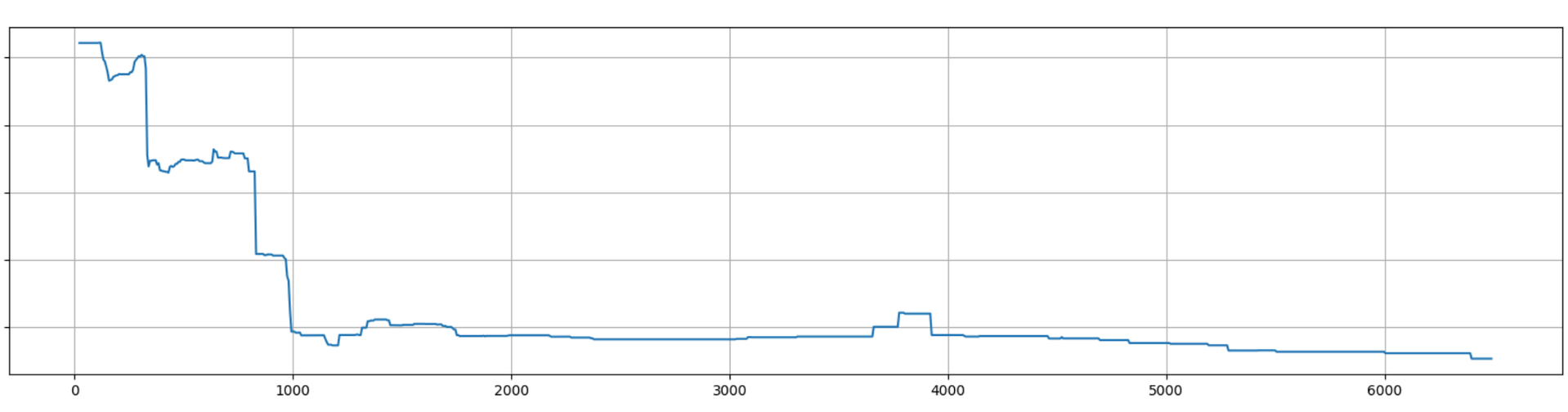


- The curve is rather smooth (despite the use of piecewise linear activations)
- Variations are relatively slow

NN vs RF Output Surface

For comparison, let's see the same response for a RF model

In [13]:
```
rf = RandomForestRegressor()
rf.fit(X_tr, y_tr.values.ravel())
rf_pred_s = rf.predict(x_sensitivity)
pred_sensitivity = pd.Series(index=a_vals, data=rf_pred_s.ravel())
pred_sensitivity.plot(figsize=figsize, grid=':');
```



- The curve is not smooth at all
- Variations can be very quick

Neural Networks and Classification

Loading and Preprocessing Data

As we mentioned, Neural network can be used for classification

We will see a practical example on the weather dataset

In [15]:
```
fname2 = os.path.join('data', 'weather.csv')
data2 = pd.read_csv(fname2, sep=',')
data2['windy'] = data2['windy'].astype('category').cat.codes
data2['play'] = data2['play'].astype('category').cat.codes
data2 = pd.get_dummies(data2, columns=['outlook'])


out_col2 = 'play'
in_cols2 = [c for c in data2.columns if c != out_col2]

X2 = data2[in_cols2].astype('float64')
y2 = data2[[out_col2]].astype('float64')
```

- We preprocess the data the same way we did for Linear regression
- We convert all features to a floating point type
- ...Since the tensorflow library expects that

Loading and Preprocessing Data

Train-test spliting and standardization are also as in Linear Regression

In [16]:
```
X_tr2, X_ts2, y_tr2, y_ts2 = train_test_split(X2, y2, test_size=0.34, random_state=42)

num_cols2 = ['temperature', 'humidity']
x_scaler = StandardScaler()
X_tr2[num_cols2] = x_scaler.fit_transform(X_tr2[num_cols2])
X_ts2[num_cols2] = x_scaler.transform(X_ts2[num_cols2])
X_tr2.head()
```

Out[16]:

	temperature	humidity	windy	outlook_overcast	outlook_rainy	outlook_sunny
8	-0.610786	-1.133519	0.0	0.0	0.0	1.0
2	1.871762	0.310965	0.0	1.0	0.0	0.0
1	1.339788	0.672087	1.0	0.0	0.0	1.0
13	-0.256136	0.762367	1.0	0.0	1.0	0.0
4	-0.788110	-0.230716	0.0	0.0	1.0	0.0

- There is no need to standardize/normalize 0-1 data
- ...Since with NNs we need normalization only to support gradient descent

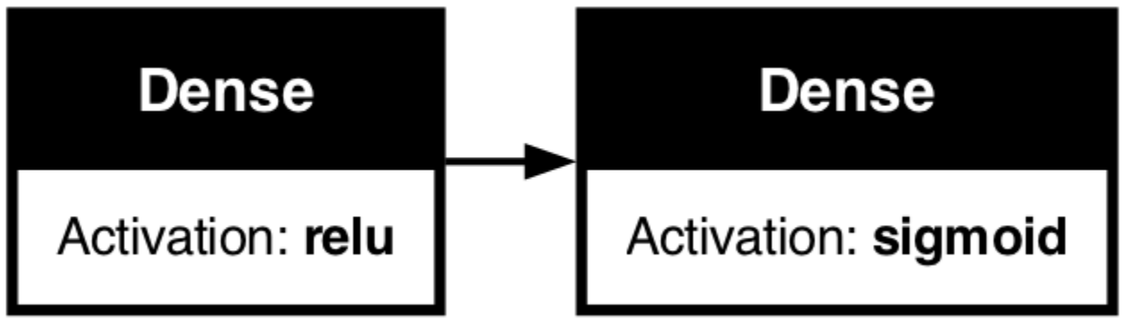
Building a Model

We need to build the network with a different output layer

In [17]:
```
input_shape2 = (len(in_cols2),)

nn2 = keras.Sequential()
nn2.add(Input(input_shape2))
nn2.add(Dense(16, activation='relu'))
nn2.add(Dense(1, activation='sigmoid'))
keras.utils.plot_model(nn2, rankdir='LR', show_layer_activations=True, dpi=150)
```

Out[17]:



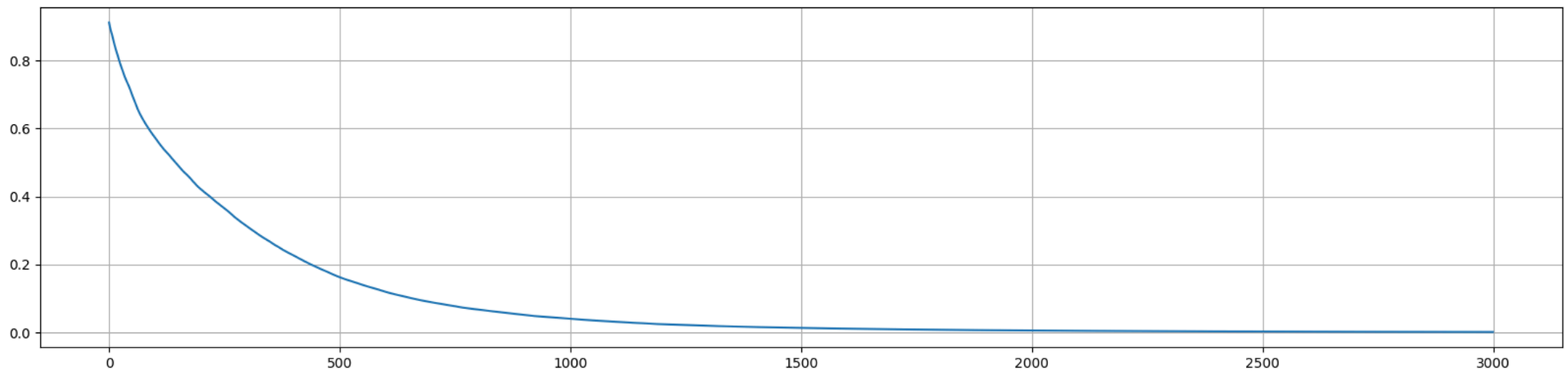
- If we have two classes, we use a sigmoid
- If we have more, we introduce one neuron per class
- ...And we pass `'sigmoid'` for the `activation` parameter

Training a Model

At training time, we need to use a different loss function

- We use `'binary_crossentropy'` with two classes
- ...And `'categorical_crossentropy'` with more classes

In [18]:
```
nn2.compile(optimizer='adam', loss='binary_crossentropy')
history2 = nn2.fit(X_tr2, y_tr2, batch_size=8, epochs=3000, verbose=0)
loss_history2 = pd.Series(name='loss', data=history2.history['loss'])
loss_history2.plot(figsize=figsize, grid=':');
```



- In our case, we need a large number of epochs since our dataset is tiny

Evaluation

Predictions are assumed to be probabilistic by default

In [19]:
```
y_pred_p_tr2 = nn2.predict(X_tr2, verbose=0)
y_pred_p_ts2 = nn2.predict(X_ts2, verbose=0)
print(y_pred_p_tr2[:3])
```

```
[[9.9999064e-01]
 [9.9974918e-01]
 [3.7887593e-04]]
```

...Se we need to use rouding to get actual classes:

In [20]:
```
y_pred_tr2 = np.round(y_pred_p_tr2)
y_pred_ts2 = np.round(y_pred_p_ts2)
print(y_pred_tr2[:3])
```

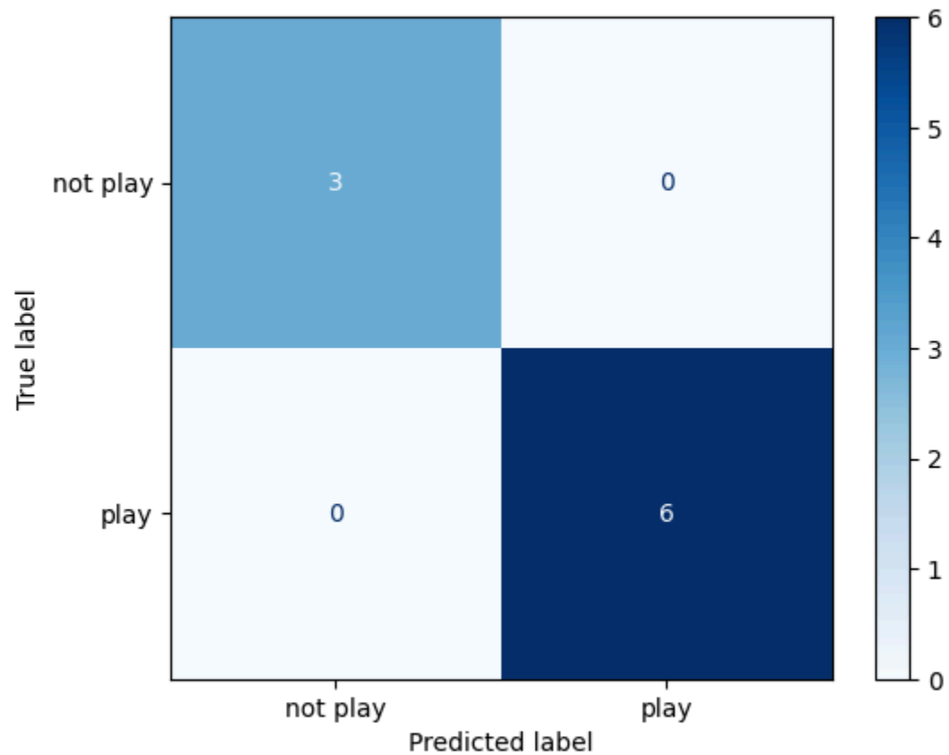
```
[[1.]
 [1.]
 [0.]]
```

Evaluation

The, we can evaluate the NN classifier as usual

In [21]:
```
from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score
print(f'Accuracy: {accuracy_score(y_tr2, y_pred_tr2):.3f} (training), {accuracy_score(y_ts2,
ConfusionMatrixDisplay.from_predictions(y_tr2, y_pred_tr2, display_labels=['not play', 'play
```

```
Accuracy: 1.000 (training), 0.400 (test)
```



Some Comments

Some observations

- Our NN results are slighly worse than those of RFs
- Training takes longer than tree based models
- ...And NN are very difficult to interpret

So, what makes NNs special?

Mostly, it's three things:

- Their ability to deal with raw input
- Their (relative) robustness w.r.t. overfitting
- Their (relative) smoothness and ability to interpolate data
- Their flexibility

We will explore these aspects in deeper detail in the next notebook