

# ex2\_sol

April 17, 2019

## 1 Exercise 2 - Introduction to (Deep) Neural Networks

This exercise uses some images and information from <https://github.com/YaleATLAS/CERNDDeepLearningTuto>

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## 3 1 Introduction to Keras

\* Modular, powerful and intuitive Deep Learning Python library built on  
and and

Developed with a focus on enabling fast experimentation. Being able to go from idea  
to result with the least possible delay is key to doing good research.

<https://keras.io>

- Minimalist, user-friendly interface
- Extremely well documented, lots of working examples
- Very shallow learning curve → by far one of the best tools for both beginners and experts
- Open-source, developed and maintained by a community of contributors, and publicly hosted on GitHub
- Extensible: possibility to customize layers

From the Keras website:

## 4 2 Breast cancer dataset

### 4.1 Loading the dataset

4.1.1 Task 1: For this exercise we want to use the breast cancer dataset from sci-kit learn. Prepare the dataset in the following way:

- Load the dataset (`load_breast_cancer`), inspect it and create a pandas DataFrame with name `df`.
- How many example and how many features do we have? What are the names of the classes? How many examples of each class do we have?
- Plot the mean radius and the mean smoothness of the training data in a 2D scatter plot for the two classes

```
In [1]: from sklearn.datasets import load_breast_cancer
```

```
breast_cancer = load_breast_cancer()
print(breast_cancer['DESCR'])
```

```
.. _breast_cancer_dataset:
```

```
Breast cancer wisconsin (diagnostic) dataset
```

```
-----
```

```
**Data Set Characteristics:**
```

```
:Number of Instances: 569
```

```
:Number of Attributes: 30 numeric, predictive attributes and the class
```

```
:Attribute Information:
```

- radius (mean of distances from center to points on the perimeter)
- texture (standard deviation of gray-scale values)
- perimeter
- area
- smoothness (local variation in radius lengths)
- compactness ( $\text{perimeter}^2 / \text{area} - 1.0$ )
- concavity (severity of concave portions of the contour)
- concave points (number of concave portions of the contour)
- symmetry
- fractal dimension ("coastline approximation" - 1)

The mean, standard error, and "worst" or largest (mean of the three largest values) of these features were computed for each image, resulting in 30 features. For instance, field 3 is Mean Radius, field 13 is Radius SE, field 23 is Worst Radius.

- class:
  - WDBC-Malignant

- WDBC-Benign

:Summary Statistics:

	Min	Max
radius (mean):	6.981	28.11
texture (mean):	9.71	39.28
perimeter (mean):	43.79	188.5
area (mean):	143.5	2501.0
smoothness (mean):	0.053	0.163
compactness (mean):	0.019	0.345
concavity (mean):	0.0	0.427
concave points (mean):	0.0	0.201
symmetry (mean):	0.106	0.304
fractal dimension (mean):	0.05	0.097
radius (standard error):	0.112	2.873
texture (standard error):	0.36	4.885
perimeter (standard error):	0.757	21.98
area (standard error):	6.802	542.2
smoothness (standard error):	0.002	0.031
compactness (standard error):	0.002	0.135
concavity (standard error):	0.0	0.396
concave points (standard error):	0.0	0.053
symmetry (standard error):	0.008	0.079
fractal dimension (standard error):	0.001	0.03
radius (worst):	7.93	36.04
texture (worst):	12.02	49.54
perimeter (worst):	50.41	251.2
area (worst):	185.2	4254.0
smoothness (worst):	0.071	0.223
compactness (worst):	0.027	1.058
concavity (worst):	0.0	1.252
concave points (worst):	0.0	0.291
symmetry (worst):	0.156	0.664
fractal dimension (worst):	0.055	0.208

:Missing Attribute Values: None

:Class Distribution: 212 - Malignant, 357 - Benign

:Creator: Dr. William H. Wolberg, W. Nick Street, Olvi L. Mangasarian

:Donor: Nick Street

:Date: November, 1995

This is a copy of UCI ML Breast Cancer Wisconsin (Diagnostic) datasets.  
<https://goo.gl/U2Uwz2>

Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

Separating plane described above was obtained using Multisurface Method-Tree (MSM-T) [K. P. Bennett, "Decision Tree Construction Via Linear Programming." Proceedings of the 4th Midwest Artificial Intelligence and Cognitive Science Society, pp. 97-101, 1992], a classification method which uses linear programming to construct a decision tree. Relevant features were selected using an exhaustive search in the space of 1-4 features and 1-3 separating planes.

The actual linear program used to obtain the separating plane in the 3-dimensional space is that described in:  
[K. P. Bennett and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets", Optimization Methods and Software 1, 1992, 23-34].

This database is also available through the UW CS ftp server:

```
ftp ftp.cs.wisc.edu
cd math-prog/cpo-dataset/machine-learn/WDBC/
```

.. topic:: References

- W.N. Street, W.H. Wolberg and O.L. Mangasarian. Nuclear feature extraction for breast tumor diagnosis. IS&T/SPIE 1993 International Symposium on Electronic Imaging: Science and Technology, volume 1905, pages 861-870, San Jose, CA, 1993.
- O.L. Mangasarian, W.N. Street and W.H. Wolberg. Breast cancer diagnosis and prognosis via linear programming. Operations Research, 43(4), pages 570-577, July-August 1995.
- W.H. Wolberg, W.N. Street, and O.L. Mangasarian. Machine learning techniques to diagnose breast cancer from fine-needle aspirates. Cancer Letters 77 (1994) 163-171.

```
In [2]: import pandas as pd
        df = pd.DataFrame(breast_cancer.data, columns=breast_cancer.feature_names)
        df.head(10)
```

```
Out[2]:    mean radius  mean texture  mean perimeter  mean area  mean smoothness  \
0         17.99         10.38         122.80        1001.0         0.11840
```

1	20.57	17.77	132.90	1326.0	0.08474
2	19.69	21.25	130.00	1203.0	0.10960
3	11.42	20.38	77.58	386.1	0.14250
4	20.29	14.34	135.10	1297.0	0.10030
5	12.45	15.70	82.57	477.1	0.12780
6	18.25	19.98	119.60	1040.0	0.09463
7	13.71	20.83	90.20	577.9	0.11890
8	13.00	21.82	87.50	519.8	0.12730
9	12.46	24.04	83.97	475.9	0.11860

	mean compactness	mean concavity	mean concave points	mean symmetry \
0	0.27760	0.30010	0.14710	0.2419
1	0.07864	0.08690	0.07017	0.1812
2	0.15990	0.19740	0.12790	0.2069
3	0.28390	0.24140	0.10520	0.2597
4	0.13280	0.19800	0.10430	0.1809
5	0.17000	0.15780	0.08089	0.2087
6	0.10900	0.11270	0.07400	0.1794
7	0.16450	0.09366	0.05985	0.2196
8	0.19320	0.18590	0.09353	0.2350
9	0.23960	0.22730	0.08543	0.2030

	mean fractal dimension	...	worst radius	worst texture	worst perimeter \
0	0.07871	...	25.38	17.33	184.60
1	0.05667	...	24.99	23.41	158.80
2	0.05999	...	23.57	25.53	152.50
3	0.09744	...	14.91	26.50	98.87
4	0.05883	...	22.54	16.67	152.20
5	0.07613	...	15.47	23.75	103.40
6	0.05742	...	22.88	27.66	153.20
7	0.07451	...	17.06	28.14	110.60
8	0.07389	...	15.49	30.73	106.20
9	0.08243	...	15.09	40.68	97.65

	worst area	worst smoothness	worst compactness	worst concavity \
0	2019.0	0.1622	0.6656	0.7119
1	1956.0	0.1238	0.1866	0.2416
2	1709.0	0.1444	0.4245	0.4504
3	567.7	0.2098	0.8663	0.6869
4	1575.0	0.1374	0.2050	0.4000
5	741.6	0.1791	0.5249	0.5355
6	1606.0	0.1442	0.2576	0.3784
7	897.0	0.1654	0.3682	0.2678
8	739.3	0.1703	0.5401	0.5390
9	711.4	0.1853	1.0580	1.1050

	worst concave points	worst symmetry	worst fractal dimension
0	0.2654	0.4601	0.11890

1	0.1860	0.2750	0.08902
2	0.2430	0.3613	0.08758
3	0.2575	0.6638	0.17300
4	0.1625	0.2364	0.07678
5	0.1741	0.3985	0.12440
6	0.1932	0.3063	0.08368
7	0.1556	0.3196	0.11510
8	0.2060	0.4378	0.10720
9	0.2210	0.4366	0.20750

[10 rows x 30 columns]

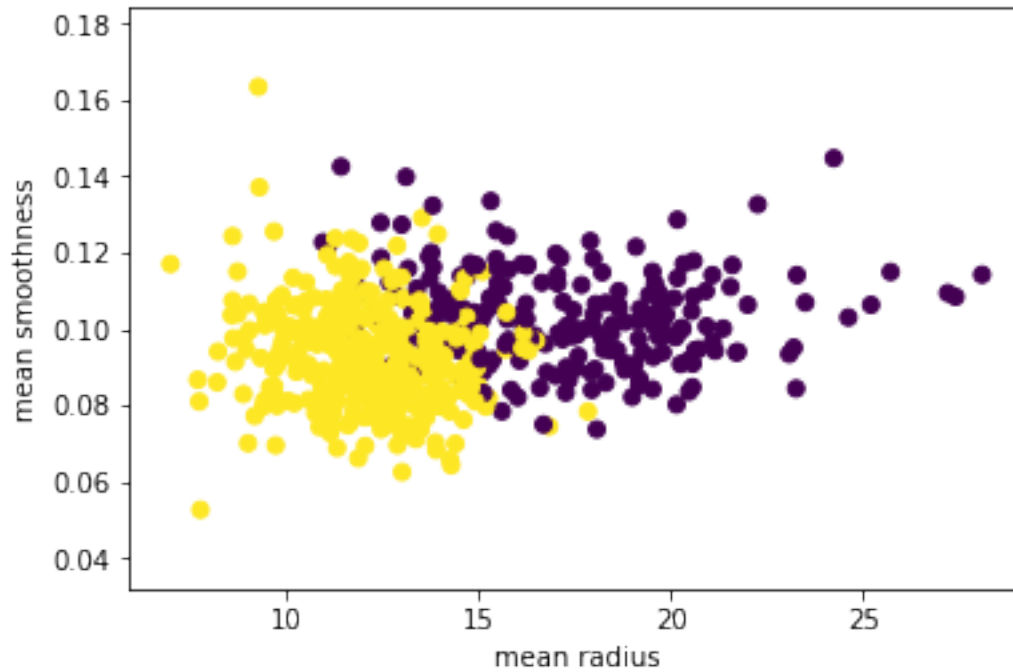
```
In [3]: import numpy as np
        print('Example number, feature number:', df.shape)
        print('Class Names:', list(breast_cancer.target_names))
        print('Class proportions:', np.bincount(breast_cancer.target))
```

```
('Example number, feature number:', (569, 30))
('Class Names:', ['malignant', 'benign'])
('Class proportions:', array([212, 357]))
```

## 4.2 Plotting the dataset

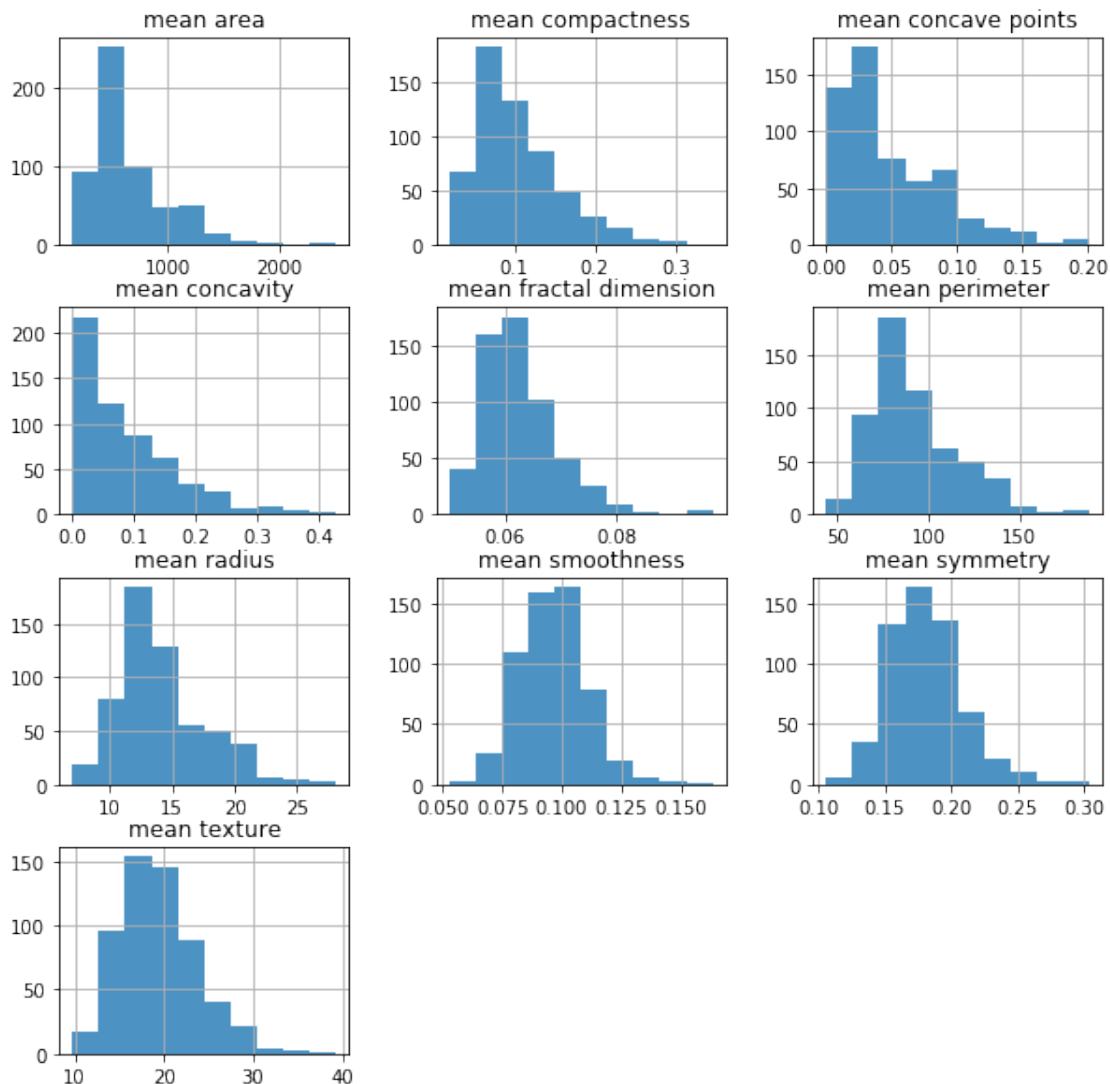
```
In [4]: %matplotlib inline
        import matplotlib.pyplot as plt
        plt.scatter(df['mean radius'], df['mean smoothness'], c=breast_cancer.target)
        plt.xlabel('mean radius')
        plt.ylabel('mean smoothness')
```

```
Out[4]: Text(0,0.5,'mean smoothness')
```



Pandas has also some nice built-in plotting features, for instance you can plot the histograms of the features:

```
In [5]: df[breast_cancer.feature_names[0:10]].hist(alpha=0.8, figsize=(10, 10))  
plt.show()
```



What if we are interested in how the shape of a distribution differs between the two classes?  
We could simply add the target to the DataFrame:

```
In [6]: df = df.assign(target=breast_cancer.target)
        df.keys()
```

```
Out[6]: Index([u'mean radius', u'mean texture', u'mean perimeter', u'mean area',
               u'mean smoothness', u'mean compactness', u'mean concavity',
               u'mean concave points', u'mean symmetry', u'mean fractal dimension',
               u'radius error', u'texture error', u'perimeter error', u'area error',
               u'smoothness error', u'compactness error', u'concavity error',
               u'concave points error', u'symmetry error', u'fractal dimension error',
               u'worst radius', u'worst texture', u'worst perimeter', u'worst area',
               u'worst smoothness', u'worst compactness', u'worst concavity',
               u'worst concave points', u'worst symmetry', u'worst fractal dimension',
```

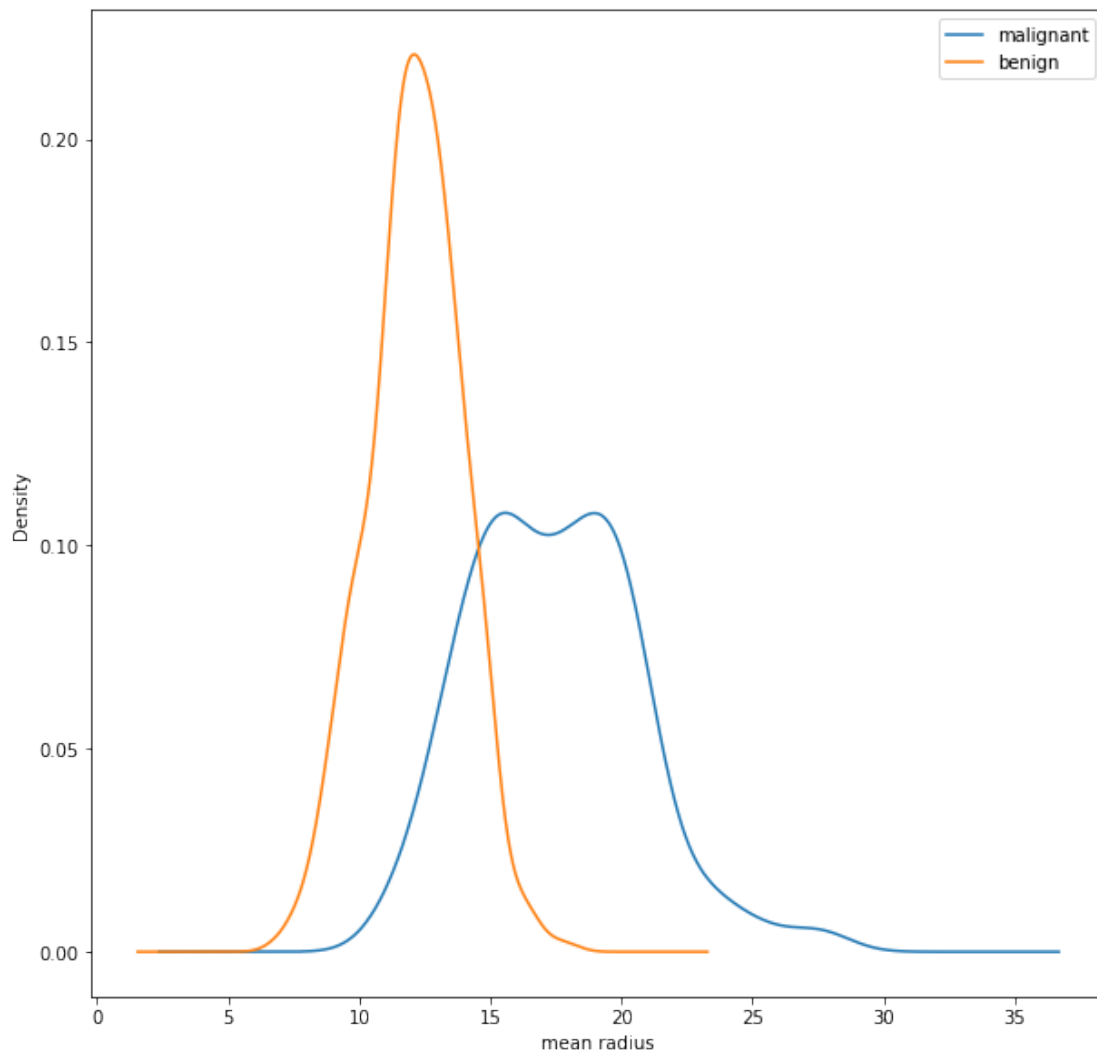


```
u'target'],  
dtype='object')
```

And then use the useful groupby function and plot a kernel density estimate (kde) plot:

```
In [7]: df.groupby("target")["mean radius"].plot(kind='kde', figsize=(10, 10))  
plt.legend(['malignant', 'benign'], loc='upper right')  
plt.xlabel('mean radius')
```

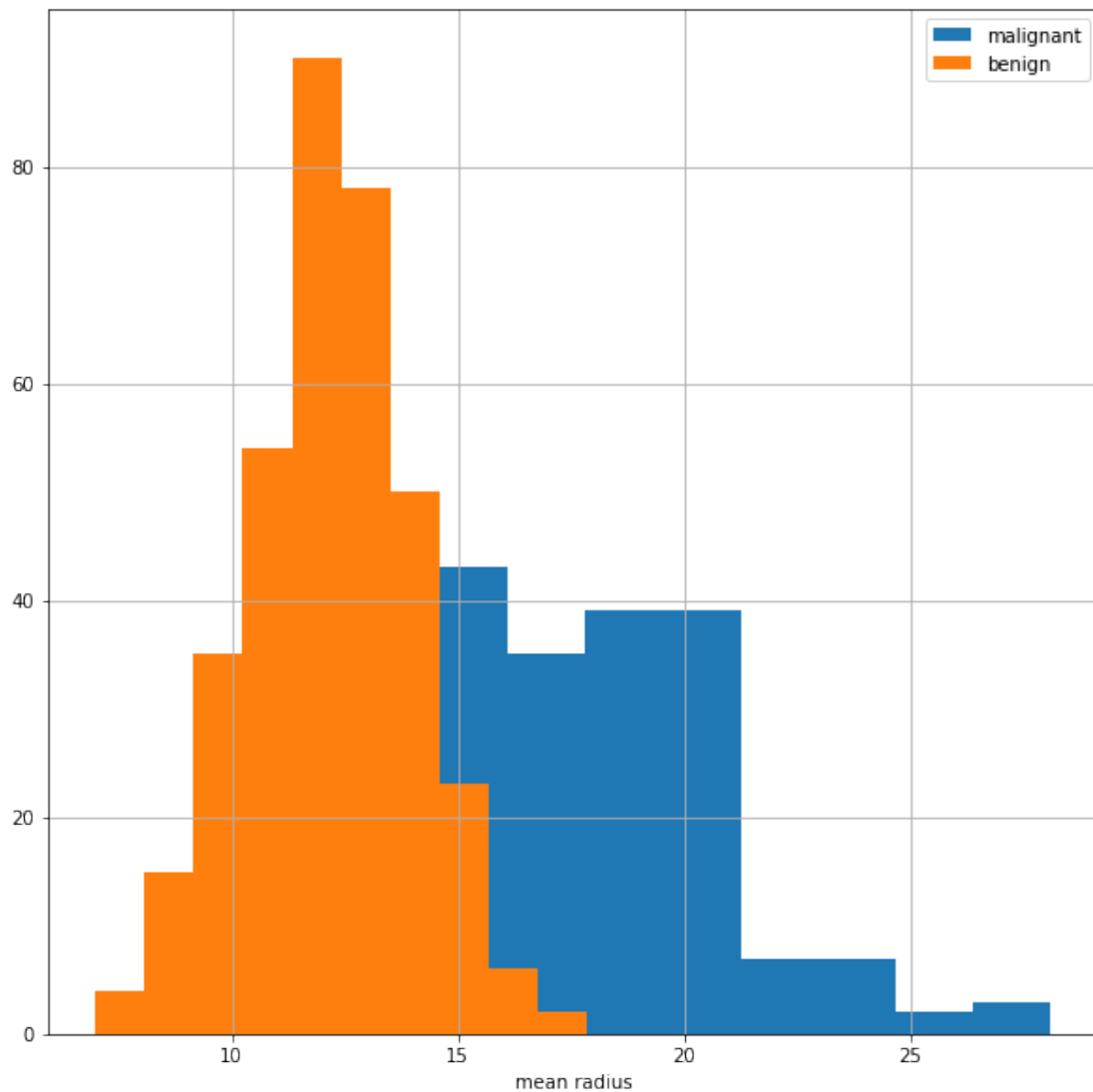
```
Out[7]: Text(0.5,0,'mean radius')
```



Similarly, we could also plot the histogram:

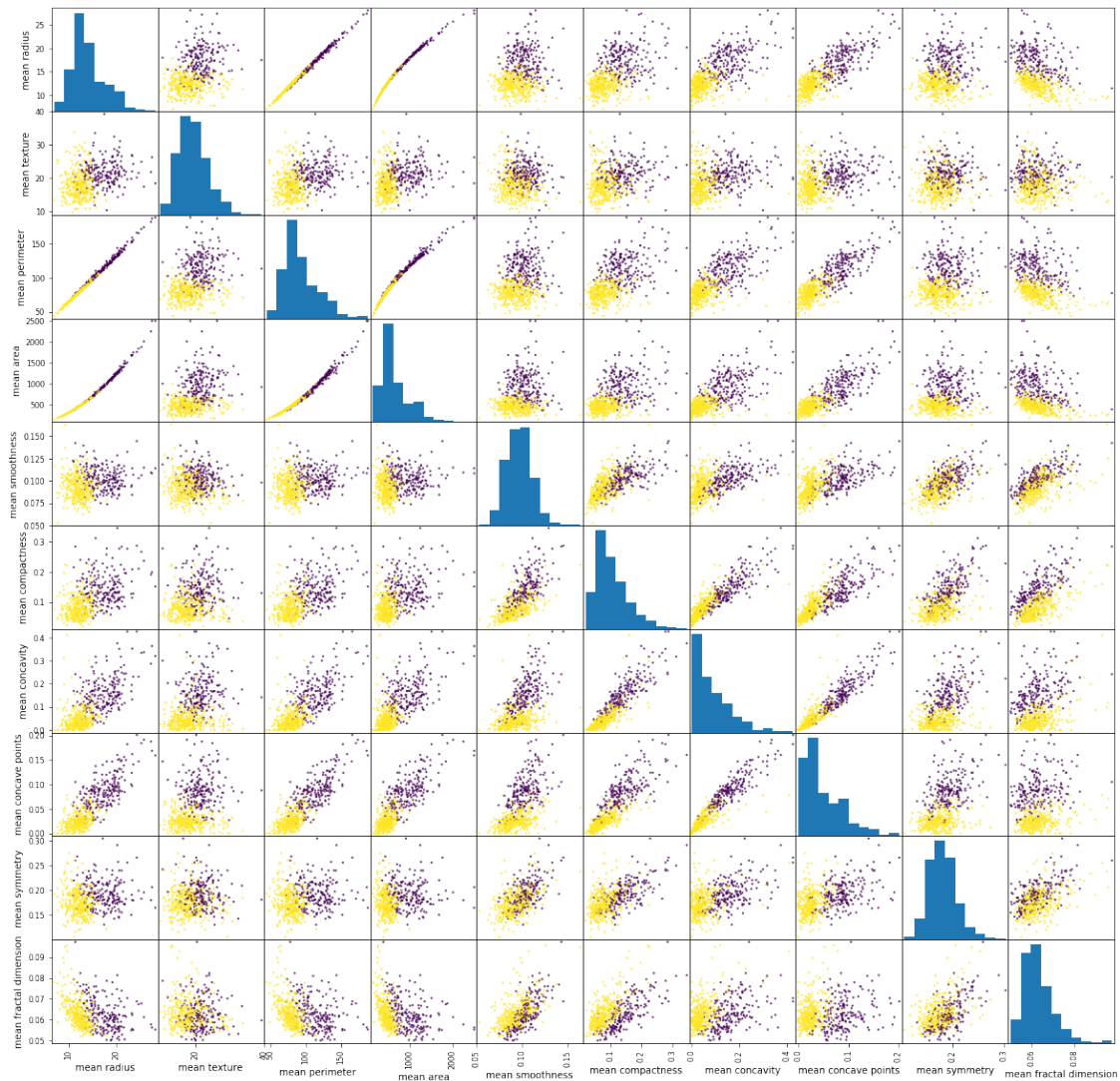
```
In [8]: df.groupby("target")["mean radius"].hist(fill=False, figsize=(10, 10))  
plt.legend(['malignant', 'benign'], loc='upper right')  
plt.xlabel('mean radius')
```

Out[8]: Text(0.5,0,'mean radius')



From a DataFrame you can even plot the full scatter plot matrix:

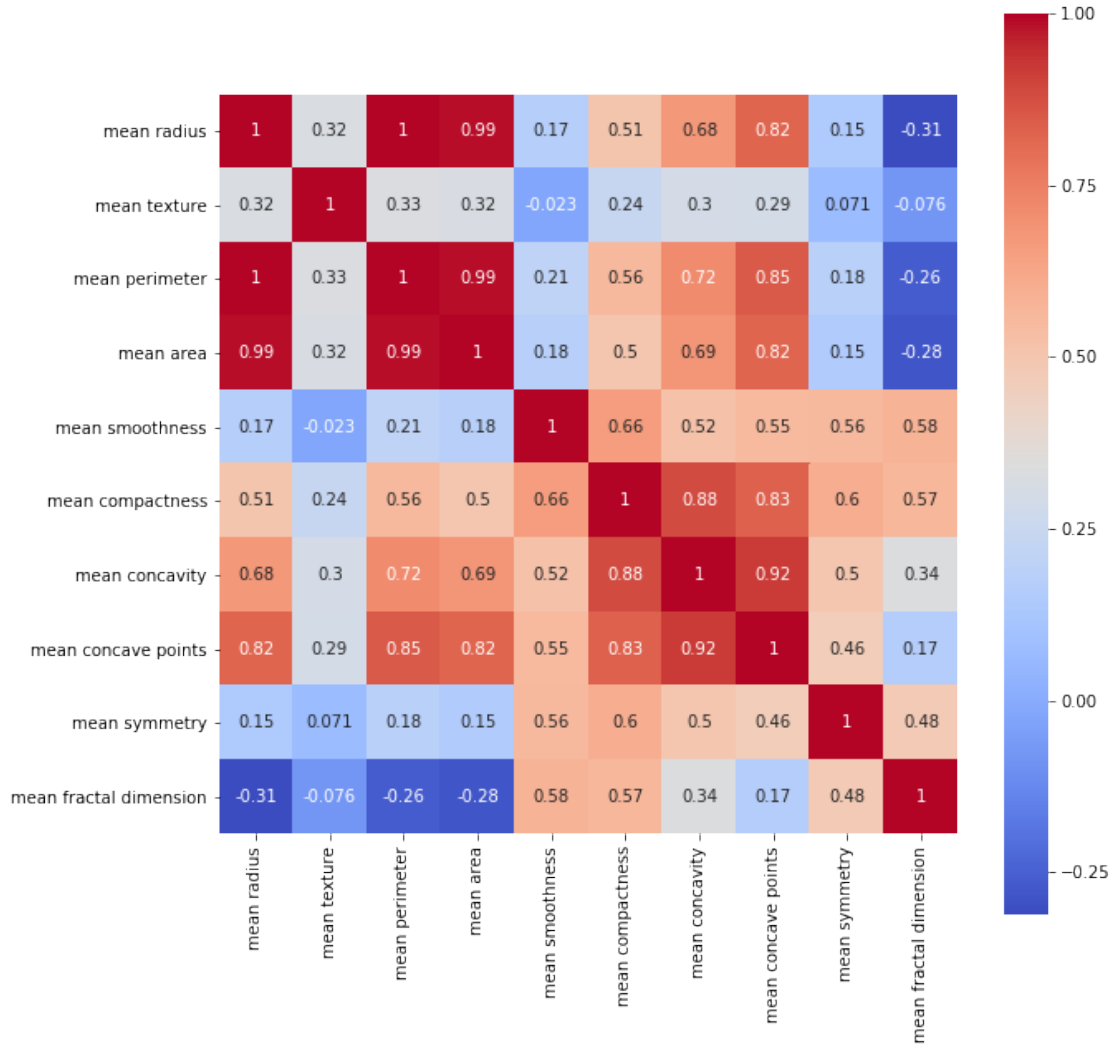
```
In [9]: from pandas.plotting import scatter_matrix
        scatter_matrix(df[breast_cancer.feature_names[0:10]], c=breast_cancer.target, alpha=0.8)
        plt.show()
```



Some of the input features seem highly correlated, so it usually makes sense to quantify their correlation to the other features. We will now use seaborn: statistical data visualization to obtain the (linear) correlations between the input features.

<https://seaborn.pydata.org/>

```
In [10]: import seaborn as sns
plt.figure(figsize=(10,10))
sns.heatmap(df[breast_cancer.feature_names[0:10]].corr(), annot=True, square=True, cm=
plt.show()
```



### 4.3 Preparing the dataset

Just like scikit-learn, Keras, takes as inputs the following objects: \*

Design matrix  $X$

an ndarray of dimensions `[nb_examples, nb_features]` containing the distributions to be used as inputs to the model. Each row is an object to classify, each column corresponds to a specific variable. \*

Target vector  $y$

an array of dimensions `[nb_examples]` containing the truth labels indicating the class each object belongs to (for classification), or the continuous target values (for regression). \*

Weight vector  $w$

(optional) an array of dimensions `[nb_examples]` containing the weights to be assigned to each example

The indices of these objects must map to the same examples.

#### 4.3.1 Task 2: Create design matrix $X$ and target vector $y$ for the first 10 features. Split the data into 70% training data and 30% testing data

```
In [11]: X = df[breast_cancer.feature_names[0:10]].values
        y = breast_cancer.target
        print('Class proportions:', np.bincount(y))
```

```
('Class proportions:', array([212, 357]))
```

```
In [12]: type(X)
```

```
Out[12]: numpy.ndarray
```

```
In [13]: X.shape
```

```
Out[13]: (569, 10)
```

```
In [14]: from sklearn.model_selection import train_test_split
        X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

        print('Class proportions:', np.bincount(y_train))
```

```
('Class proportions:', array([148, 250]))
```

It is common practice to scale the inputs to neural nets such that they have approximately similar ranges. Without this step, you might end up with variables whose values span very different orders of magnitude. This will create problems in the NN convergence due to very wild fluctuations in the magnitude of the internal weights. To take care of the scaling, we use the sklearn StandardScaler:

```
In [15]: from sklearn.preprocessing import StandardScaler
```

```
In [16]: scaler = StandardScaler()
        X_train = scaler.fit_transform(X_train)
        X_test = scaler.transform(X_test)
```

## 5 3 Training a dense neural network

### 5.1 Neural network model

#### 5.1.1 Dense layer structure

- Densely connected layer, where all inputs are connected to all outputs
- Linear transformation of the input vector  $x \in \mathbb{R}^n$ , which can be expressed using the  $n \times m$  matrix  $W \in \mathbb{R}^{n \times m}$  as:

$$u = Wx + b$$

where  $b \in \mathbb{R}^m$  is the bias unit

- All entries in both  $W$  and  $b$  are trainable

- In Keras: 

```
keras.layers.Dense(units,
activation=None, use_bias=True, kernel_initializer='glorot',
bias_initializer='zeros', kernel_regularizer=None, bias_regularizer=None,
activity_regularizer=None, kernel_constraint=None,
bias_constraint=None )
```

- `input_dim` (or `input_shape`) are necessary arguments for the 1st layer of the net:

“python # as first layer in a sequential model: `model = Sequential() model.add(Dense(32, input_shape=(16,)))` # now the model will take as input arrays of shape `(, 16)` # and output arrays of shape `(, 32)`

## 6 after the first layer, you don't need to specify

## 7 the size of the input anymore:

`model.add(Dense(32))` “

### 7.0.1 Activation functions

- Mathematical way of quantifying the activation state of a node → whether it's firing or not
- Non-linear activation functions are the key to Deep Learning
- Allow NNs to learn complex, non-linear transformations of the inputs
- Some popular choices:

Available activations: \* `softmax`, `elu`, `selu`, `softplus`, `softsign`, `relu`, `tanh`, `sigmoid`, `hard_sigmoid`, `linear`

Advanced Activation: \* `LeakyReLU`, `PReLU`

### 7.0.2 Loss functions

- Mathematical way of quantifying how much  $y$  deviates from  $y$
- Dictates how strongly we penalize certain types of mistakes
- Cost of inaccurately classifying an event
- Many loss functions available in Keras (<https://keras.io/losses/>)

## 7.1 Build a simple neural network

In [23]: `from keras.models import Sequential`

`model = Sequential()`

In [24]: `from keras.layers import Dense`

In [25]: `model.add(Dense(units=11, activation='relu', input_dim=10))`  
`model.add(Dense(units=1, activation='sigmoid'))`

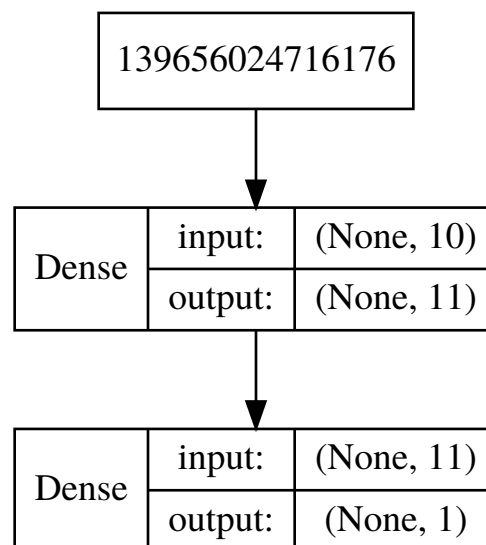
```
In [26]: model.summary()
```

```
-----
Layer (type)                 Output Shape              Param #
=====
dense_5 (Dense)              (None, 11)                121
-----
dense_6 (Dense)              (None, 1)                 12
=====
Total params: 133
Trainable params: 133
Non-trainable params: 0
-----
```

Let's visualize our net:

```
In [27]: from IPython.display import SVG, Image
         from keras.utils.vis_utils import model_to_dot, plot_model
         SVG(model_to_dot(model, show_shapes=True, show_layer_names=False).create(prog='dot',
         #Or as an image:
         #from keras.utils.vis_utils import plot_model
         #plot_model(model, to_file='model_plot.png', show_shapes=True, show_layer_names=False,
         #Image('model_plot.png'))
```

Out [27]:



Another nice tool is ANNvisualizer: <https://github.com/Prodicode/ann-visualizer>

```
In [28]: from ann_visualizer.visualize import ann_viz;
         ann_viz(model, view=True, filename="network.gv", title="Shallow Network")
```

OK, that is a rather simple model, but let's define a loss function, an optimizer, a performance metric and compile it:

```
In [29]: model.compile(loss='binary_crossentropy',
                        optimizer='sgd',
                        metrics=['accuracy'])
```

### 7.1.1 Training

In order to train the model, we pass the training data to the fit function. However, part of the training data will be used as validation data, which is used during the training to evaluate the training process.

```
In [30]: # x_train and y_train are Numpy arrays --just like in the Scikit-Learn API.
         history = model.fit(X_train, y_train, validation_split=0.3, epochs=100, batch_size=8)
```

WARNING:tensorflow:From /home/nackenho/miniconda/envs/TUDortmundMLSeminar/lib/python2.7/site-p

Instructions for updating:

Use tf.cast instead.

Train on 278 samples, validate on 120 samples

Epoch 1/100

278/278 [=====] - 1s 3ms/step - loss: 0.8316 - acc: 0.3813 - val\_loss

Epoch 2/100

278/278 [=====] - 0s 407us/step - loss: 0.6204 - acc: 0.6007 - val\_loss

Epoch 3/100

278/278 [=====] - 0s 333us/step - loss: 0.5211 - acc: 0.7014 - val\_loss

Epoch 4/100

278/278 [=====] - 0s 388us/step - loss: 0.4629 - acc: 0.7734 - val\_loss

Epoch 5/100

278/278 [=====] - 0s 342us/step - loss: 0.4225 - acc: 0.8453 - val\_loss

Epoch 6/100

278/278 [=====] - 0s 379us/step - loss: 0.3917 - acc: 0.8813 - val\_loss

Epoch 7/100

278/278 [=====] - 0s 357us/step - loss: 0.3662 - acc: 0.9029 - val\_loss

Epoch 8/100

278/278 [=====] - 0s 315us/step - loss: 0.3442 - acc: 0.9101 - val\_loss

Epoch 9/100

278/278 [=====] - 0s 666us/step - loss: 0.3243 - acc: 0.9209 - val\_loss

Epoch 10/100

278/278 [=====] - 0s 462us/step - loss: 0.3061 - acc: 0.9245 - val\_loss

Epoch 11/100

278/278 [=====] - 0s 397us/step - loss: 0.2893 - acc: 0.9281 - val\_loss

Epoch 12/100

278/278 [=====] - 0s 491us/step - loss: 0.2735 - acc: 0.9388 - val\_loss

Epoch 13/100

278/278 [=====] - 0s 328us/step - loss: 0.2597 - acc: 0.9353 - val\_loss

Epoch 14/100

278/278 [=====] - 0s 569us/step - loss: 0.2477 - acc: 0.9353 - val\_loss

Epoch 15/100



278/278 [=====] - 0s 689us/step - loss: 0.2373 - acc: 0.9353 - val\_loss: 0.2373  
 Epoch 16/100  
 278/278 [=====] - 0s 547us/step - loss: 0.2281 - acc: 0.9353 - val\_loss: 0.2281  
 Epoch 17/100  
 278/278 [=====] - 0s 418us/step - loss: 0.2203 - acc: 0.9353 - val\_loss: 0.2203  
 Epoch 18/100  
 278/278 [=====] - 0s 445us/step - loss: 0.2134 - acc: 0.9353 - val\_loss: 0.2134  
 Epoch 19/100  
 278/278 [=====] - 0s 412us/step - loss: 0.2074 - acc: 0.9317 - val\_loss: 0.2074  
 Epoch 20/100  
 278/278 [=====] - 0s 401us/step - loss: 0.2022 - acc: 0.9317 - val\_loss: 0.2022  
 Epoch 21/100  
 278/278 [=====] - 1s 2ms/step - loss: 0.1975 - acc: 0.9317 - val\_loss: 0.1975  
 Epoch 22/100  
 278/278 [=====] - 0s 829us/step - loss: 0.1934 - acc: 0.9317 - val\_loss: 0.1934  
 Epoch 23/100  
 278/278 [=====] - 0s 322us/step - loss: 0.1898 - acc: 0.9317 - val\_loss: 0.1898  
 Epoch 24/100  
 278/278 [=====] - 0s 398us/step - loss: 0.1865 - acc: 0.9317 - val\_loss: 0.1865  
 Epoch 25/100  
 278/278 [=====] - 0s 308us/step - loss: 0.1836 - acc: 0.9317 - val\_loss: 0.1836  
 Epoch 26/100  
 278/278 [=====] - 0s 322us/step - loss: 0.1807 - acc: 0.9317 - val\_loss: 0.1807  
 Epoch 27/100  
 278/278 [=====] - 0s 323us/step - loss: 0.1781 - acc: 0.9317 - val\_loss: 0.1781  
 Epoch 28/100  
 278/278 [=====] - 0s 338us/step - loss: 0.1759 - acc: 0.9353 - val\_loss: 0.1759  
 Epoch 29/100  
 278/278 [=====] - 0s 441us/step - loss: 0.1736 - acc: 0.9388 - val\_loss: 0.1736  
 Epoch 30/100  
 278/278 [=====] - 0s 524us/step - loss: 0.1715 - acc: 0.9388 - val\_loss: 0.1715  
 Epoch 31/100  
 278/278 [=====] - 0s 410us/step - loss: 0.1694 - acc: 0.9388 - val\_loss: 0.1694  
 Epoch 32/100  
 278/278 [=====] - 0s 651us/step - loss: 0.1676 - acc: 0.9424 - val\_loss: 0.1676  
 Epoch 33/100  
 278/278 [=====] - 0s 637us/step - loss: 0.1658 - acc: 0.9424 - val\_loss: 0.1658  
 Epoch 34/100  
 278/278 [=====] - 0s 623us/step - loss: 0.1642 - acc: 0.9388 - val\_loss: 0.1642  
 Epoch 35/100  
 278/278 [=====] - 0s 630us/step - loss: 0.1625 - acc: 0.9424 - val\_loss: 0.1625  
 Epoch 36/100  
 278/278 [=====] - 0s 470us/step - loss: 0.1611 - acc: 0.9424 - val\_loss: 0.1611  
 Epoch 37/100  
 278/278 [=====] - 0s 558us/step - loss: 0.1596 - acc: 0.9424 - val\_loss: 0.1596  
 Epoch 38/100  
 278/278 [=====] - 0s 512us/step - loss: 0.1583 - acc: 0.9496 - val\_loss: 0.1583  
 Epoch 39/100

278/278 [=====] - 0s 317us/step - loss: 0.1570 - acc: 0.9496 - val\_loss: 0.1570  
 Epoch 40/100  
 278/278 [=====] - 0s 457us/step - loss: 0.1558 - acc: 0.9496 - val\_loss: 0.1558  
 Epoch 41/100  
 278/278 [=====] - 0s 593us/step - loss: 0.1545 - acc: 0.9496 - val\_loss: 0.1545  
 Epoch 42/100  
 278/278 [=====] - 0s 1ms/step - loss: 0.1533 - acc: 0.9496 - val\_loss: 0.1533  
 Epoch 43/100  
 278/278 [=====] - 0s 581us/step - loss: 0.1522 - acc: 0.9496 - val\_loss: 0.1522  
 Epoch 44/100  
 278/278 [=====] - 0s 456us/step - loss: 0.1511 - acc: 0.9496 - val\_loss: 0.1511  
 Epoch 45/100  
 278/278 [=====] - 0s 1ms/step - loss: 0.1499 - acc: 0.9496 - val\_loss: 0.1499  
 Epoch 46/100  
 278/278 [=====] - 0s 1ms/step - loss: 0.1490 - acc: 0.9460 - val\_loss: 0.1490  
 Epoch 47/100  
 278/278 [=====] - 0s 643us/step - loss: 0.1480 - acc: 0.9460 - val\_loss: 0.1480  
 Epoch 48/100  
 278/278 [=====] - 0s 456us/step - loss: 0.1471 - acc: 0.9460 - val\_loss: 0.1471  
 Epoch 49/100  
 278/278 [=====] - 0s 543us/step - loss: 0.1461 - acc: 0.9460 - val\_loss: 0.1461  
 Epoch 50/100  
 278/278 [=====] - 0s 371us/step - loss: 0.1451 - acc: 0.9460 - val\_loss: 0.1451  
 Epoch 51/100  
 278/278 [=====] - 0s 608us/step - loss: 0.1442 - acc: 0.9460 - val\_loss: 0.1442  
 Epoch 52/100  
 278/278 [=====] - 0s 428us/step - loss: 0.1433 - acc: 0.9460 - val\_loss: 0.1433  
 Epoch 53/100  
 278/278 [=====] - 0s 409us/step - loss: 0.1425 - acc: 0.9460 - val\_loss: 0.1425  
 Epoch 54/100  
 278/278 [=====] - 0s 624us/step - loss: 0.1416 - acc: 0.9496 - val\_loss: 0.1416  
 Epoch 55/100  
 278/278 [=====] - 0s 511us/step - loss: 0.1409 - acc: 0.9496 - val\_loss: 0.1409  
 Epoch 56/100  
 278/278 [=====] - 0s 536us/step - loss: 0.1400 - acc: 0.9496 - val\_loss: 0.1400  
 Epoch 57/100  
 278/278 [=====] - 0s 554us/step - loss: 0.1393 - acc: 0.9496 - val\_loss: 0.1393  
 Epoch 58/100  
 278/278 [=====] - 0s 479us/step - loss: 0.1386 - acc: 0.9532 - val\_loss: 0.1386  
 Epoch 59/100  
 278/278 [=====] - 0s 364us/step - loss: 0.1378 - acc: 0.9532 - val\_loss: 0.1378  
 Epoch 60/100  
 278/278 [=====] - 0s 1ms/step - loss: 0.1372 - acc: 0.9532 - val\_loss: 0.1372  
 Epoch 61/100  
 278/278 [=====] - 0s 327us/step - loss: 0.1364 - acc: 0.9532 - val\_loss: 0.1364  
 Epoch 62/100  
 278/278 [=====] - 0s 295us/step - loss: 0.1358 - acc: 0.9532 - val\_loss: 0.1358  
 Epoch 63/100

278/278 [=====] - 0s 372us/step - loss: 0.1352 - acc: 0.9532 - val\_loss: 0.1352  
 Epoch 64/100  
 278/278 [=====] - 0s 313us/step - loss: 0.1346 - acc: 0.9640 - val\_loss: 0.1346  
 Epoch 65/100  
 278/278 [=====] - 0s 404us/step - loss: 0.1340 - acc: 0.9604 - val\_loss: 0.1340  
 Epoch 66/100  
 278/278 [=====] - 0s 376us/step - loss: 0.1333 - acc: 0.9604 - val\_loss: 0.1333  
 Epoch 67/100  
 278/278 [=====] - 0s 299us/step - loss: 0.1327 - acc: 0.9640 - val\_loss: 0.1327  
 Epoch 68/100  
 278/278 [=====] - 0s 239us/step - loss: 0.1322 - acc: 0.9640 - val\_loss: 0.1322  
 Epoch 69/100  
 278/278 [=====] - 0s 353us/step - loss: 0.1315 - acc: 0.9640 - val\_loss: 0.1315  
 Epoch 70/100  
 278/278 [=====] - 0s 347us/step - loss: 0.1310 - acc: 0.9640 - val\_loss: 0.1310  
 Epoch 71/100  
 278/278 [=====] - 0s 210us/step - loss: 0.1304 - acc: 0.9676 - val\_loss: 0.1304  
 Epoch 72/100  
 278/278 [=====] - 0s 411us/step - loss: 0.1300 - acc: 0.9676 - val\_loss: 0.1300  
 Epoch 73/100  
 278/278 [=====] - 0s 206us/step - loss: 0.1294 - acc: 0.9676 - val\_loss: 0.1294  
 Epoch 74/100  
 278/278 [=====] - 0s 298us/step - loss: 0.1289 - acc: 0.9676 - val\_loss: 0.1289  
 Epoch 75/100  
 278/278 [=====] - 0s 326us/step - loss: 0.1284 - acc: 0.9676 - val\_loss: 0.1284  
 Epoch 76/100  
 278/278 [=====] - 0s 379us/step - loss: 0.1278 - acc: 0.9676 - val\_loss: 0.1278  
 Epoch 77/100  
 278/278 [=====] - 0s 375us/step - loss: 0.1273 - acc: 0.9676 - val\_loss: 0.1273  
 Epoch 78/100  
 278/278 [=====] - 0s 329us/step - loss: 0.1268 - acc: 0.9676 - val\_loss: 0.1268  
 Epoch 79/100  
 278/278 [=====] - 0s 403us/step - loss: 0.1264 - acc: 0.9640 - val\_loss: 0.1264  
 Epoch 80/100  
 278/278 [=====] - 0s 443us/step - loss: 0.1259 - acc: 0.9676 - val\_loss: 0.1259  
 Epoch 81/100  
 278/278 [=====] - 0s 426us/step - loss: 0.1255 - acc: 0.9640 - val\_loss: 0.1255  
 Epoch 82/100  
 278/278 [=====] - 0s 374us/step - loss: 0.1250 - acc: 0.9640 - val\_loss: 0.1250  
 Epoch 83/100  
 278/278 [=====] - 0s 355us/step - loss: 0.1245 - acc: 0.9640 - val\_loss: 0.1245  
 Epoch 84/100  
 278/278 [=====] - 0s 383us/step - loss: 0.1241 - acc: 0.9640 - val\_loss: 0.1241  
 Epoch 85/100  
 278/278 [=====] - 0s 406us/step - loss: 0.1236 - acc: 0.9640 - val\_loss: 0.1236  
 Epoch 86/100  
 278/278 [=====] - 0s 413us/step - loss: 0.1232 - acc: 0.9640 - val\_loss: 0.1232  
 Epoch 87/100

```

278/278 [=====] - 0s 339us/step - loss: 0.1228 - acc: 0.9676 - val_loss: 0.1228
Epoch 88/100
278/278 [=====] - 0s 320us/step - loss: 0.1224 - acc: 0.9640 - val_loss: 0.1224
Epoch 89/100
278/278 [=====] - 0s 537us/step - loss: 0.1219 - acc: 0.9640 - val_loss: 0.1219
Epoch 90/100
278/278 [=====] - 0s 342us/step - loss: 0.1215 - acc: 0.9676 - val_loss: 0.1215
Epoch 91/100
278/278 [=====] - 0s 428us/step - loss: 0.1211 - acc: 0.9676 - val_loss: 0.1211
Epoch 92/100
278/278 [=====] - 0s 392us/step - loss: 0.1207 - acc: 0.9676 - val_loss: 0.1207
Epoch 93/100
278/278 [=====] - 0s 364us/step - loss: 0.1204 - acc: 0.9676 - val_loss: 0.1204
Epoch 94/100
278/278 [=====] - 0s 483us/step - loss: 0.1199 - acc: 0.9676 - val_loss: 0.1199
Epoch 95/100
278/278 [=====] - 0s 515us/step - loss: 0.1195 - acc: 0.9676 - val_loss: 0.1195
Epoch 96/100
278/278 [=====] - 0s 519us/step - loss: 0.1192 - acc: 0.9676 - val_loss: 0.1192
Epoch 97/100
278/278 [=====] - 0s 415us/step - loss: 0.1188 - acc: 0.9676 - val_loss: 0.1188
Epoch 98/100
278/278 [=====] - 0s 419us/step - loss: 0.1185 - acc: 0.9676 - val_loss: 0.1185
Epoch 99/100
278/278 [=====] - 0s 526us/step - loss: 0.1181 - acc: 0.9676 - val_loss: 0.1181
Epoch 100/100
278/278 [=====] - 0s 412us/step - loss: 0.1178 - acc: 0.9676 - val_loss: 0.1178

```

During the training process we have saved the loss and the accuracy of the training and validation data:

```

In [31]: print(history.history.keys())

['acc', 'loss', 'val_acc', 'val_loss']

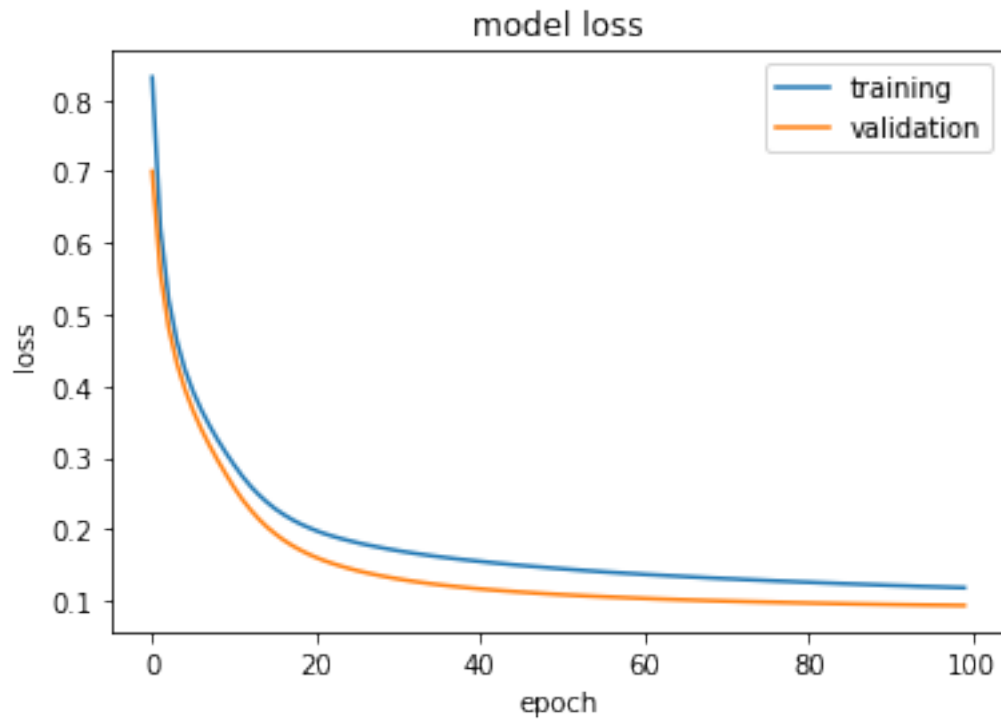
```

We can now plot the loss evolution over the training epochs for the training and validation dataset:

```

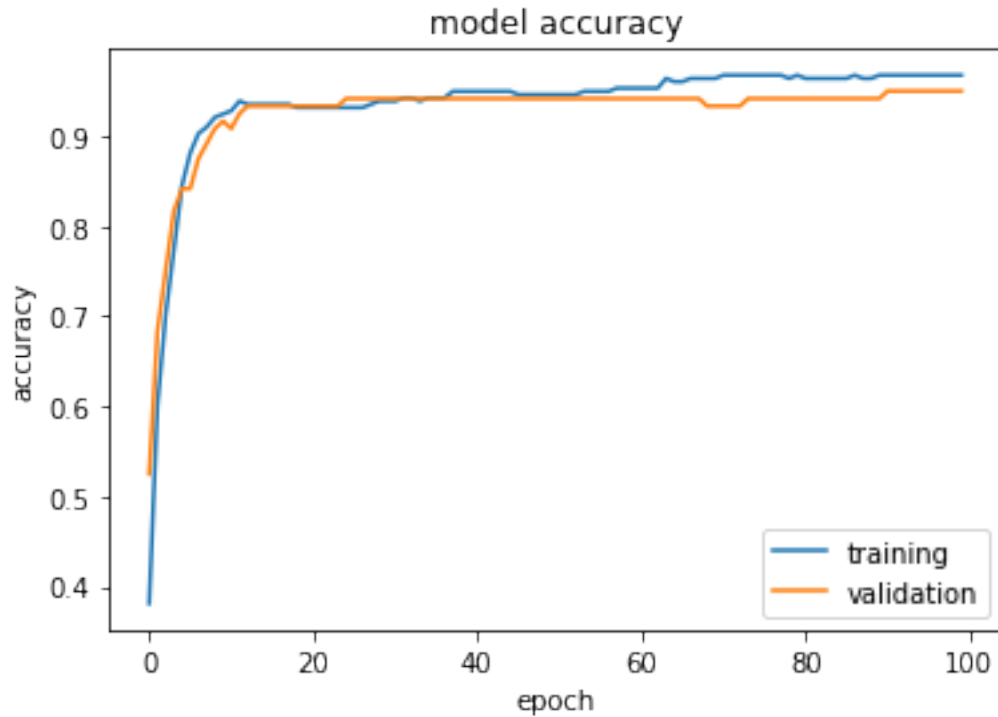
In [32]: # summarize history for loss
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('model loss')
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['training', 'validation'], loc='upper right')
plt.show()

```



Similarly, we can plot the accuracy

```
In [33]: # summarize history for accuracy
plt.plot(history.history['acc'])
plt.plot(history.history['val_acc'])
plt.title('model accuracy')
plt.ylabel('accuracy')
plt.xlabel('epoch')
plt.legend(['training', 'validation'], loc='lower right')
plt.show()
```



### 7.1.2 Evaluation

Let's evaluate the loss and accuracy on our test data:

```
In [34]: loss_and_metrics = model.evaluate(X_test, y_test, batch_size=8)
         print loss_and_metrics
```

```
171/171 [=====] - 0s 227us/step
[0.1589359859255148, 0.9356725147941656]
```

Let's predict classes for our test data:

```
In [35]: print 'Testing...'
         y_pred = model.predict(X_test, verbose = True, batch_size=8)
```

```
Testing...
171/171 [=====] - 0s 419us/step
```

```
In [36]: # predictions
         y_pred
```

```
Out[36]: array([[2.0281255e-02],
               [4.6252140e-01],
               [7.8973299e-01],
               [3.5119057e-04],
               [7.9836607e-02],
               [8.7759495e-03],
               [9.9997735e-01],
               [1.5273419e-01],
               [9.8745799e-01],
               [0.0000000e+00],
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               [9.8729229e-01],
               [1.0742846e-01],
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               [9.9635220e-01],
               [8.6256385e-01],
               [4.0991306e-03],
               [5.7660431e-02],
               [9.3278837e-01],
               [9.8385620e-01],
               [8.8267696e-01],
               [9.5441788e-01],
               [9.5916253e-01],
               [3.6860406e-03],
               [1.6125679e-02],
               [9.1045254e-01],
               [9.9548542e-01],
               [9.8359358e-01],
               [7.3269010e-04],
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               [9.0348673e-01],
               [1.2455612e-02],
               [6.6323799e-01],
               [9.9898273e-01],
               [4.0364265e-04],
               [9.5258629e-01],
               [7.9508263e-01],
               [9.4850969e-01],
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               [9.4928074e-01],
               [6.8882716e-01],
               [9.9826157e-03],
               [9.9847203e-01],
               [9.9965870e-01],
               [9.3850303e-01],
               [4.7511008e-01],
               [3.5564333e-01],
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[4.1630566e-03],  
[5.1855445e-03],

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[8.9406967e-08],
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[3.4521580e-02],
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[9.8751116e-01],
[1.8118322e-03],
[9.9908400e-01],
[9.9203205e-01],
[9.9975324e-01],
[2.9595464e-01],
[9.1934162e-01],
[9.8888063e-01]], dtype=float32)

```

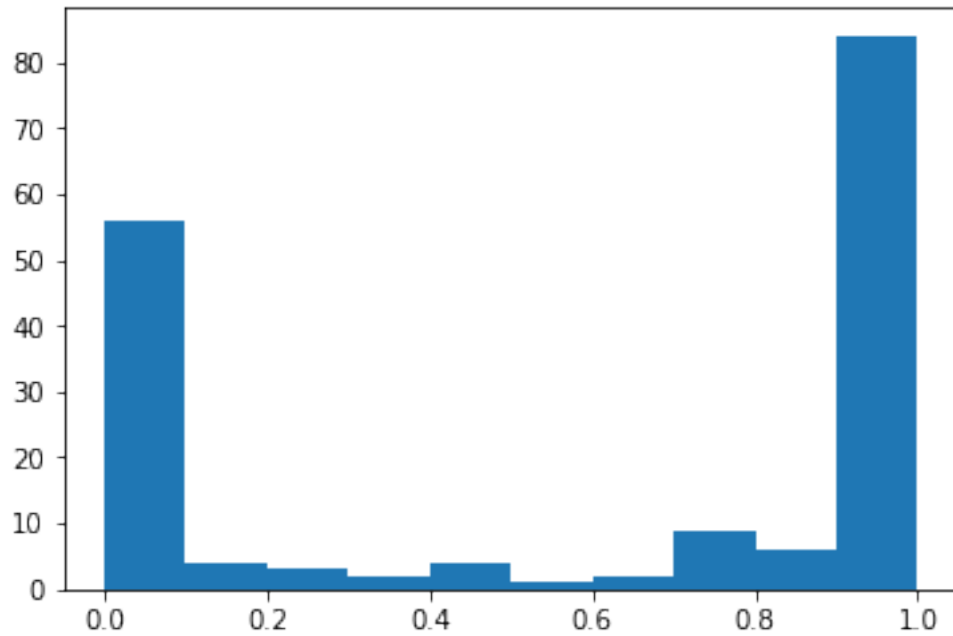
### 7.1.3 Task 3: Plot the output prediction for malignant and benign breast cancer showing the separation between these two classes.

```
In [37]: plt.hist(y_pred)
```

```

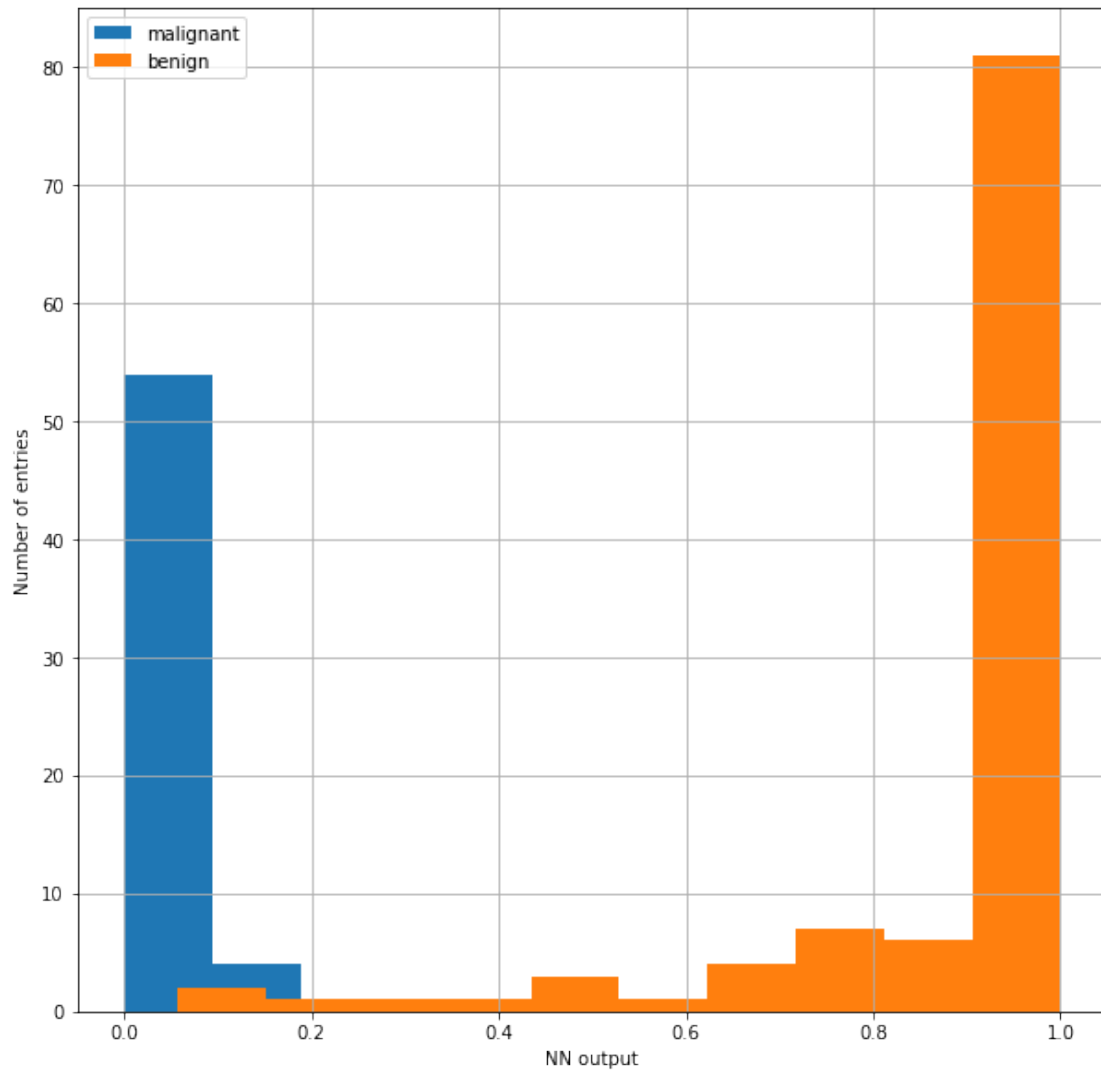
Out[37]: (array([56.,  4.,  3.,  2.,  4.,  1.,  2.,  9.,  6., 84.]),
          array([0.          , 0.0999985 , 0.19999701, 0.2999955 , 0.39999402,
                0.49999252, 0.599991  , 0.69998956, 0.79998803, 0.8999865 ,
                0.99998504], dtype=float32),
          <a list of 10 Patch objects>)

```



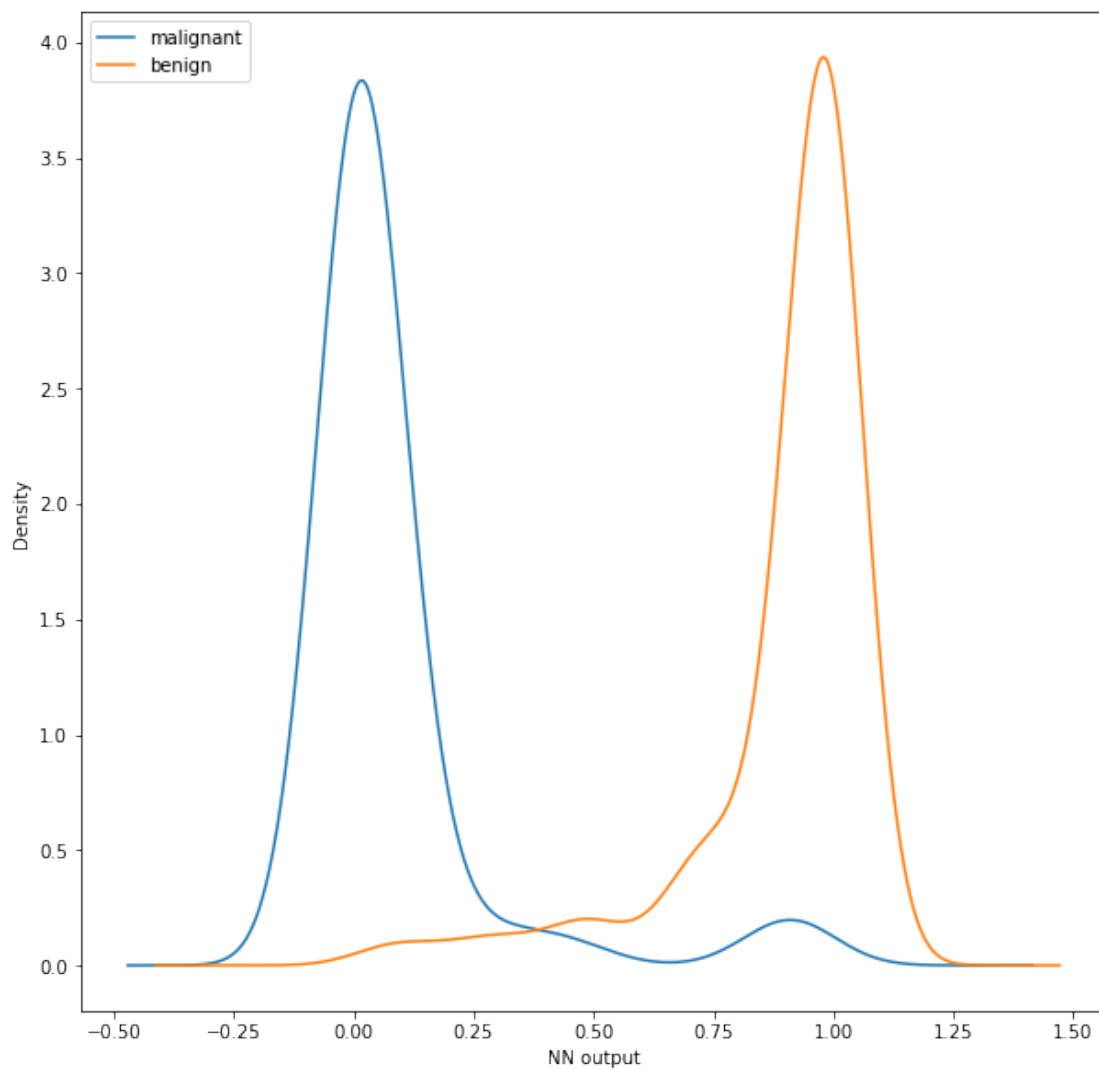
```
In [38]: nn_out = pd.DataFrame()
nn_out = nn_out.assign(prediction = y_pred.ravel())
nn_out = nn_out.assign(target = y_test)
nn_out.groupby("target")["prediction"].hist(normed=1,figsize=(10, 10))
plt.legend(['malignant', 'benign'], loc='upper left')
plt.xlabel('NN output')
plt.ylabel('Number of entries')
```

```
Out[38]: Text(0,0.5,'Number of entries')
```



```
In [39]: nn_out = pd.DataFrame()
nn_out = nn_out.assign(prediction = y_pred.ravel())
nn_out = nn_out.assign(target = y_test)
nn_out.groupby("target")["prediction"].plot(kind='kde', figsize=(10, 10))
plt.legend(['malignant', 'benign'], loc='upper left')
plt.xlabel('NN output')
plt.ylabel('Density')
```

```
Out[39]: Text(0,0.5,'Density')
```



How do we decide now to which class the test example needs to assigned based on our prediction? Intuitively, we could simply convert our predictions into classes by using a threshold of 0.5:

```
In [40]: y_cls=np.where(y_pred > 0.5, 1, 0)
         print y_cls
```

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```
In [41]: y_cls = model.predict_classes(X_test, batch_size=1)
         print y_cls
```

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#### 7.1.4 Task 4: Use the scikit learn metrics to evaluate the model

```
In [42]: from sklearn.metrics import accuracy_score, precision_score, recall_score, classification_report  
         print('Accuracy: %.2f' % accuracy_score(y_test, y_cls))  
         print("Precision: %.2f" % precision_score(y_test, y_cls, average='weighted'))  
         print("Recall: %.2f" % recall_score(y_test, y_cls, average='weighted'))  
         print 'Classification Report:\n', classification_report(y_test, y_cls)
```

Accuracy: 0.94

Precision: 0.94

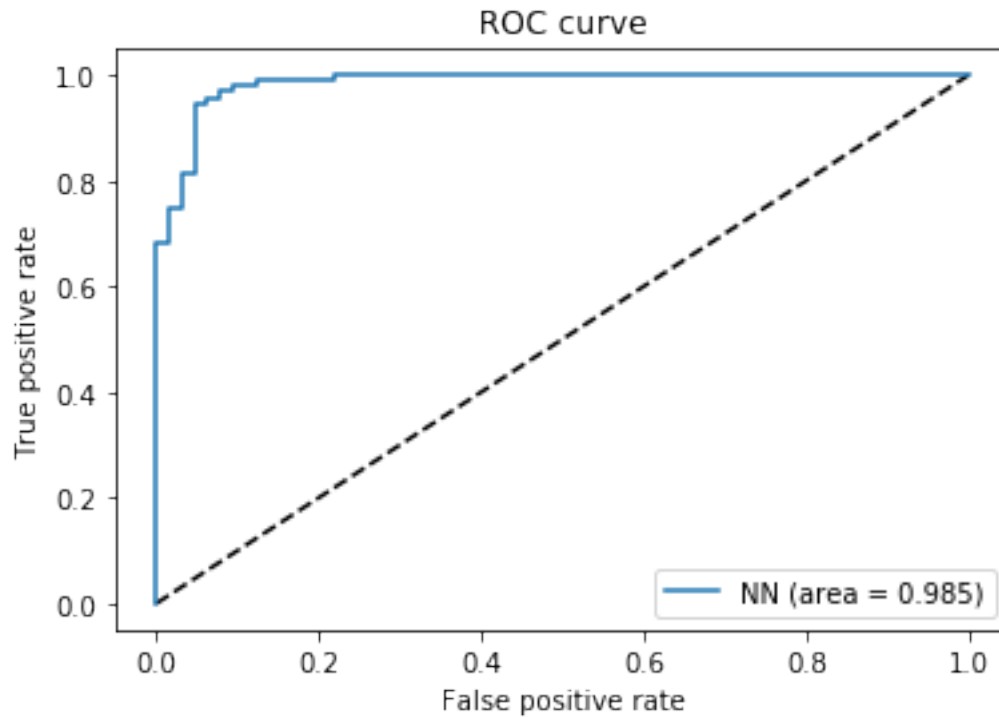
Recall: 0.94

Classification Report:

	precision	recall	f1-score	support
0	0.88	0.95	0.92	64
1	0.97	0.93	0.95	107
micro avg	0.94	0.94	0.94	171
macro avg	0.93	0.94	0.93	171
weighted avg	0.94	0.94	0.94	171

Now, let's use scikit learn also to plot the ROC curve and calculate the AUC:

```
In [43]: from sklearn.metrics import roc_curve, auc  
         fpr, tpr, thresholds = roc_curve(y_test, y_pred.ravel())  
         auc = auc(fpr, tpr)  
         plt.figure(1)  
         plt.plot([0, 1], [0, 1], 'k--')  
         plt.plot(fpr, tpr, label='NN (area = {:.3f})'.format(auc))  
         plt.xlabel('False positive rate')  
         plt.ylabel('True positive rate')  
         plt.title('ROC curve')  
         plt.legend(loc='best')  
         plt.show()
```



## 7.2 Task 5 (Bonus): Change the neural network model and study the impact on the performance

- Make the neural network wider
- Make the neural network deeper
- Change the activation function of the hidden nodes
- Change the activation function of the output node
- Change the loss function, which ones are allowed?
- Which neural network gives the best performance?