ex3_sol

April 24, 2019

1 Exercise 3 - Input Scaling and Regularization

Part of this exercise is taken from http://scikit-learn.org/stable/auto_examples/preprocessing/plot_all_scaling.

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3 Loading the dataset

- 3.0.1 Task 1: For this exercise we want to use the california housing dataset from scikit learn. Prepare the dataset in the following way:
 - Load the dataset (fetch_california_housing), inspect it and create a pandas DataFrame with name df.
 - What kind of problem is this?
 - How many example and how many features do we have? What are the features? What is the target?
 - How does the target look like?
 - Make 2D scatter plots of all input features, where the z-axis shows the target dependence.
 - What do you observe?

:Number of Instances: 20640

:Number of Attributes: 8 numeric, predictive attributes and the target

:Attribute Information:

MedInc median income in block
 HouseAge median house age in block
 AveRooms average number of rooms
 AveBedrms average number of bedrooms

- Population block population

AveOccup average house occupancyLatitude house block latitudeLongitude house block longitude

:Missing Attribute Values: None

This dataset was obtained from the StatLib repository. http://lib.stat.cmu.edu/datasets/

The target variable is the median house value for California districts.

This dataset was derived from the 1990 U.S. census, using one row per census block group. A block group is the smallest geographical unit for which the U.S. Census Bureau publishes sample data (a block group typically has a population of 600 to 3,000 people).

It can be downloaded/loaded using the :func:`sklearn.datasets.fetch_california_housing` function.

.. topic:: References

- Pace, R. Kelley and Ronald Barry, Sparse Spatial Autoregressions, Statistics and Probability Letters, 33 (1997) 291-297

In [2]: import pandas as pd

df = pd.DataFrame(housing.data, columns=housing.feature_names)
df.head(10)

Out[2]:	${\tt MedInc}$	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	\
0	8.3252	41.0	6.984127	1.023810	322.0	2.555556	37.88	
1	8.3014	21.0	6.238137	0.971880	2401.0	2.109842	37.86	
2	7.2574	52.0	8.288136	1.073446	496.0	2.802260	37.85	
3	5.6431	52.0	5.817352	1.073059	558.0	2.547945	37.85	
4	3.8462	52.0	6.281853	1.081081	565.0	2.181467	37.85	
5	4.0368	52.0	4.761658	1.103627	413.0	2.139896	37.85	

6	3.6591	52.0	4.931907	0.951362	1094.0	2.128405	37.84
7	3.1200	52.0	4.797527	1.061824	1157.0	1.788253	37.84
8	2.0804	42.0	4.294118	1.117647	1206.0	2.026891	37.84
9	3.6912	52.0	4.970588	0.990196	1551.0	2.172269	37.84

Longitude

0 -122.23

1 -122.22

2 -122.24

3 -122.25

4 -122.25

5 -122.25

6 -122.25

7 -122.25

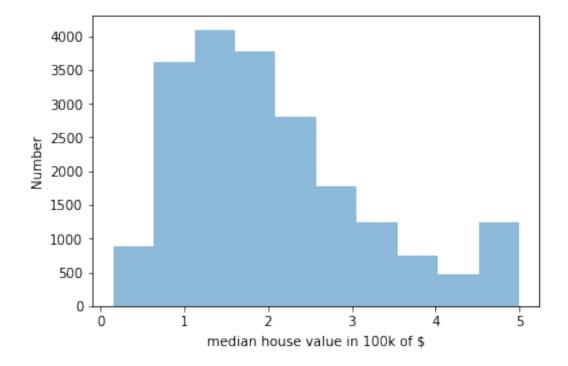
8 -122.26

9 -122.25

In [3]: %matplotlib inline

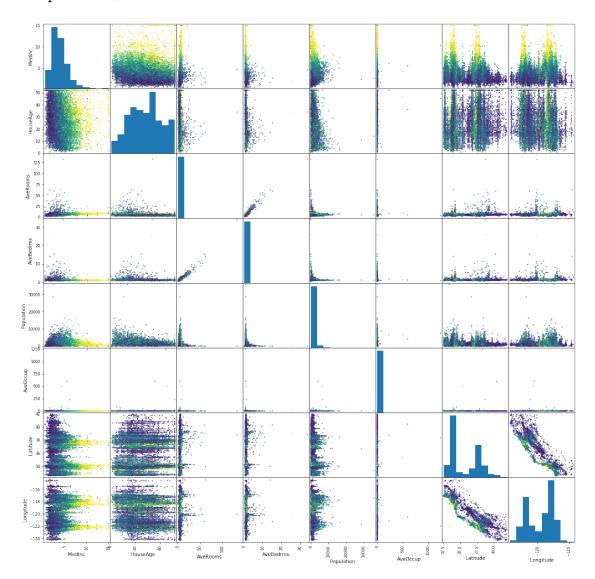
import matplotlib.pyplot as plt
plt.hist(housing.target, alpha=0.5)
plt.xlabel('median house value in 100k of \$')
plt.ylabel('Number')

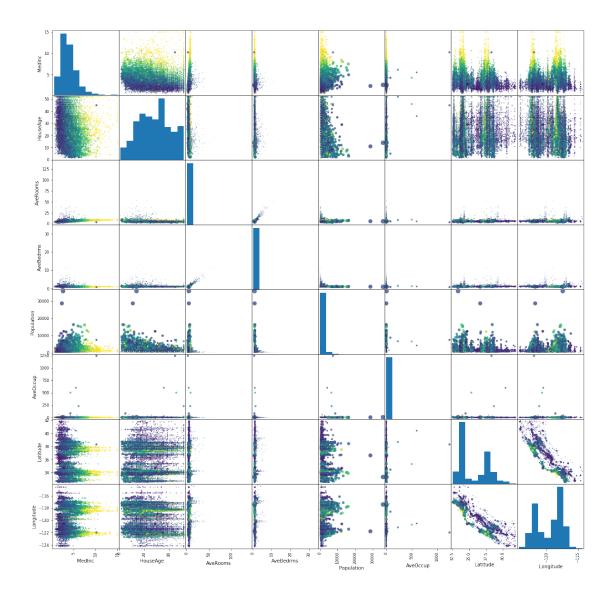
Out[3]: Text(0,0.5,'Number')



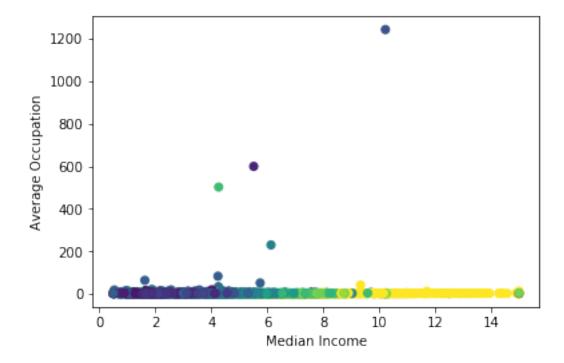
In [4]: df.shape

Out[4]: (20640, 8)





4 Comparison of different input scaling



Feature 0 (median income in a block) and feature 5 (number of households) of the California housing dataset have very different scales and contain some very large outliers. These two characteristics lead to difficulties to visualize the data and, more importantly, they can degrade the predictive performance of many machine learning algorithms. Unscaled data can also slow down or even prevent the convergence of many gradient-based estimators.

Indeed many estimators are designed with the assumption that each feature takes values close to zero or more importantly that all features vary on comparable scales. In particular, metric-based and gradient-based estimators often assume approximately standardized data (centered features with unit variances). A notable exception are decision tree-based estimators that are robust to arbitrary scaling of the data.

This example uses different scalers, transformers, and normalizers to bring the data within a pre-defined range.

Scalers are linear (or more precisely affine) transformers and differ from each other in the way to estimate the parameters used to shift and scale each feature.

QuantileTransformer provides a non-linear transformation in which distances between marginal outliers and inliers are shrunk.

Unlike the previous transformations, normalization refers to a per sample transformation instead of a per feature transformation.

4.1 Scaling the target

```
In [8]: housing.target
Out[8]: array([4.526, 3.585, 3.521, ..., 0.923, 0.847, 0.894])
```

It often makes sense to scale the target of a regression to something between 0 and 1, because that way you can use activation functions in the output layer which map to that range. If you use functions like sigmoid in the output layer, this keeps the backpropagated error within limits, unlike the case of unbounded linear activation functions. You could even scale to ranges like [0.3, 0.7] in order to focus on the almost linear-part of the sigmoid function. In the following we will scale the target between 0 and 1 also for plotting reasons. We will use the minmax_scale for that

4.2 Scaling the input

We will focus in the following on the median income [0] and number of households [5] scatter plot and how different scalings impact their range.

```
In [10]: X = housing.data[:, [0, 5]]
```

In the following, I have taken the scaling and plotting code from http://scikit-learn.org/stable/auto_examples/preprocessing/plot_all_scaling.html#results.

You don't need to understand how the scaling and plotting is done for now, but the purpose is mainly to demonstrate how different scalers impact your input

```
In [11]: # Author: Raghav RV <rvraghav93@gmail.com>
                   Guillaume Lemaitre <q.lemaitre58@qmail.com>
                    Thomas Unterthiner
         # License: BSD 3 clause
         import numpy as np
         import matplotlib as mpl
         from matplotlib import pyplot as plt
         from matplotlib import cm
         from sklearn.preprocessing import MinMaxScaler
         from sklearn.preprocessing import MaxAbsScaler
         from sklearn.preprocessing import StandardScaler
         from sklearn.preprocessing import RobustScaler
         from sklearn.preprocessing import Normalizer
         from sklearn.preprocessing.data import QuantileTransformer
         distributions = \Gamma
             ('Unscaled data', X),
             ('Data after standard scaling',
                 StandardScaler().fit_transform(X)),
```

```
('Data after min-max scaling',
                 MinMaxScaler().fit_transform(X)),
             ('Data after max-abs scaling',
                 MaxAbsScaler().fit_transform(X)),
             ('Data after robust scaling',
                 RobustScaler(quantile_range=(25, 75)).fit_transform(X)),
             ('Data after quantile transformation (uniform pdf)',
                 QuantileTransformer(output_distribution='uniform')
                 .fit transform(X)),
             ('Data after quantile transformation (gaussian pdf)',
                 QuantileTransformer(output_distribution='normal')
                 .fit_transform(X)),
             ('Data after sample-wise L2 normalizing',
                 Normalizer().fit_transform(X))
         ]
In [12]: def create_axes(title, figsize=(16, 6)):
             fig = plt.figure(figsize=figsize)
             fig.suptitle(title)
             # define the axis for the first plot
             left, width = 0.1, 0.22
             bottom, height = 0.1, 0.7
             bottom_h = height + 0.15
             left h = left + width + 0.02
             rect_scatter = [left, bottom, width, height]
             rect_histx = [left, bottom_h, width, 0.1]
             rect_histy = [left_h, bottom, 0.05, height]
             ax_scatter = plt.axes(rect_scatter)
             ax_histx = plt.axes(rect_histx)
             ax_histy = plt.axes(rect_histy)
             # define the axis for the zoomed-in plot
             left = width + left + 0.2
             left_h = left + width + 0.02
             rect_scatter = [left, bottom, width, height]
             rect histx = [left, bottom h, width, 0.1]
             rect_histy = [left_h, bottom, 0.05, height]
             ax_scatter_zoom = plt.axes(rect_scatter)
             ax_histx_zoom = plt.axes(rect_histx)
             ax_histy_zoom = plt.axes(rect_histy)
             # define the axis for the colorbar
             left, width = width + left + 0.13, 0.01
```

```
rect_colorbar = [left, bottom, width, height]
    ax_colorbar = plt.axes(rect_colorbar)
    return ((ax scatter, ax histy, ax histx),
            (ax_scatter_zoom, ax_histy_zoom, ax_histx_zoom),
            ax colorbar)
def plot_distribution(axes, X, y, hist_nbins=50, title="",
                      x0_label="", x1_label=""):
    ax, hist_X1, hist_X0 = axes
    ax.set_title(title)
    ax.set_xlabel(x0_label)
    ax.set_ylabel(x1_label)
    # The scatter plot
    colors = cm.plasma_r(y)
    ax.scatter(X[:, 0], X[:, 1], alpha=0.5, marker='o', s=5, lw=0, c=colors)
    # Removing the top and the right spine for aesthetics
    # make nice axis layout
    ax.spines['top'].set_visible(False)
    ax.spines['right'].set_visible(False)
    ax.get_xaxis().tick_bottom()
    ax.get_yaxis().tick_left()
    ax.spines['left'].set_position(('outward', 10))
    ax.spines['bottom'].set_position(('outward', 10))
    # Histogram for axis X1 (feature 5)
    hist_X1.set_ylim(ax.get_ylim())
    hist_X1.hist(X[:, 1], bins=hist_nbins, orientation='horizontal',
                 color='grey', ec='grey')
    hist X1.axis('off')
    # Histogram for axis XO (feature 0)
    hist_X0.set_xlim(ax.get_xlim())
    hist_X0.hist(X[:, 0], bins=hist_nbins, orientation='vertical',
                 color='grey', ec='grey')
    hist_X0.axis('off')
```

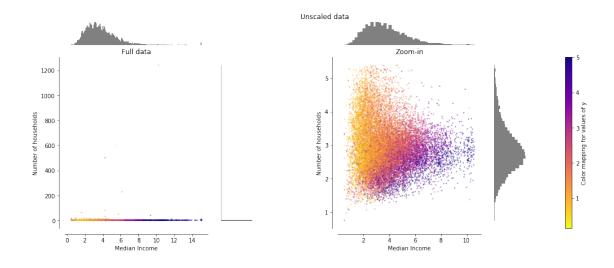
Two plots will be shown for each scaler/normalizer/transformer. The left figure will show a scatter plot of the full data set while the right figure will exclude the extreme values considering only 99 % of the data set, excluding marginal outliers. In addition, the marginal distributions for each feature will be shown on the side of the scatter plot.

```
ax_zoom_out, ax_zoom_in, ax_colorbar = create_axes(title)
axarr = (ax_zoom_out, ax_zoom_in)
plot_distribution(axarr[0], X, y, hist_nbins=200,
                  x0_label="Median Income",
                  x1 label="Number of households",
                  title="Full data")
# zoom-in
zoom_in_percentile_range = (0, 99)
cutoffs_X0 = np.percentile(X[:, 0], zoom_in_percentile_range)
cutoffs_X1 = np.percentile(X[:, 1], zoom_in_percentile_range)
non_outliers_mask = (
    np.all(X > [cutoffs_X0[0], cutoffs_X1[0]], axis=1) &
    np.all(X < [cutoffs_X0[1], cutoffs_X1[1]], axis=1))</pre>
plot_distribution(axarr[1], X[non_outliers_mask], y[non_outliers_mask],
                  hist_nbins=50,
                  x0_label="Median Income",
                  x1_label="Number of households",
                  title="Zoom-in")
norm = mpl.colors.Normalize(y_full.min(), y_full.max())
mpl.colorbar.ColorbarBase(ax_colorbar, cmap=cm.plasma_r,
                          norm=norm, orientation='vertical',
                          label='Color mapping for values of y')
```

4.3 Original data

Each transformation is plotted showing two transformed features, with the left plot showing the entire dataset, and the right zoomed-in to show the dataset without the marginal outliers. A large majority of the samples are compacted to a specific range, [0, 10] for the median income and [0, 6] for the number of households. Note that there are some marginal outliers (some blocks have more than 1200 households). Therefore, a specific pre-processing can be very beneficial depending of the application. In the following, we present some insights and behaviors of those pre-processing methods in the presence of marginal outliers.

```
In [14]: make_plot(0)
```

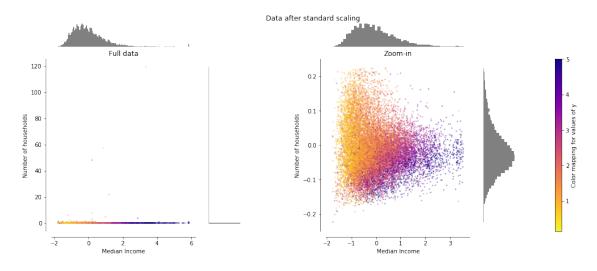


4.4 StandardScaler

StandardScaler removes the mean (0) and scales the data to unit variance (1). However, the outliers have an influence when computing the empirical mean and standard deviation which shrink the range of the feature values as shown in the left figure below. Note in particular that because the outliers on each feature have different magnitudes, the spread of the transformed data on each feature is very different: most of the data lie in the [-2, 4] range for the transformed median income feature while the same data is squeezed in the smaller [-0.2, 0.2] range for the transformed number of households.

StandardScaler therefore cannot guarantee balanced feature scales in the presence of outliers.

In [15]: make_plot(1)

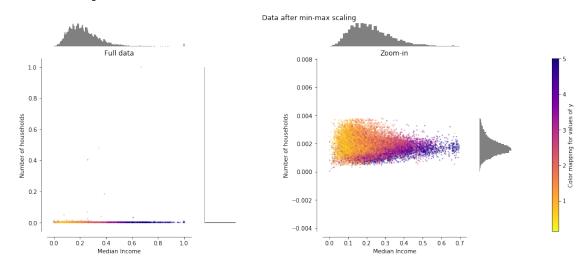


4.5 MinMaxScaler

MinMaxScaler rescales the data set such that all feature values are in the range [0, 1] as shown in the right panel below. However, this scaling compress all inliers in the narrow range [0, 0.005] for the transformed number of households.

As StandardScaler, MinMaxScaler is very sensitive to the presence of outliers.

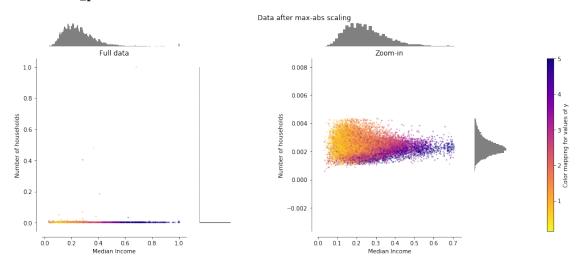
In [16]: make_plot(2)



4.6 MaxAbsScaler

MaxAbsScaler differs from the previous scaler such that the absolute values are mapped in the range [0, 1]. On positive only data, this scaler behaves similarly to MinMaxScaler and therefore also suffers from the presence of large outliers.

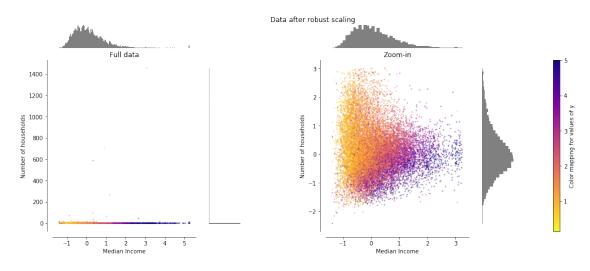
In [17]: make_plot(3)



4.7 RobustScaler

Unlike the previous scalers, the centering and scaling statistics of this scaler are based on percentiles and are therefore not influenced by a few number of very large marginal outliers. Consequently, the resulting range of the transformed feature values is larger than for the previous scalers and, more importantly, are approximately similar: for both features most of the transformed values lie in a [-2, 3] range as seen in the zoomed-in figure. Note that the outliers themselves are still present in the transformed data. If a separate outlier clipping is desirable, a non-linear transformation is required (see below).

In [18]: make_plot(4)

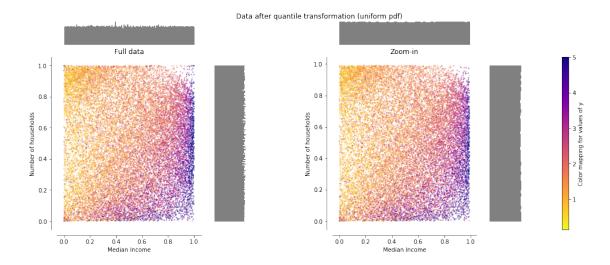


4.8 QuantileTransformer (uniform output)

QuantileTransformer applies a non-linear transformation such that the probability density function of each feature will be mapped to a uniform distribution. In this case, all the data will be mapped in the range [0, 1], even the outliers which cannot be distinguished anymore from the inliers.

As RobustScaler, QuantileTransformer is robust to outliers in the sense that adding or removing outliers in the training set will yield approximately the same transformation on held out data. But contrary to RobustScaler, QuantileTransformer will also automatically collapse any outlier by setting them to the a priori defined range boundaries (0 and 1).

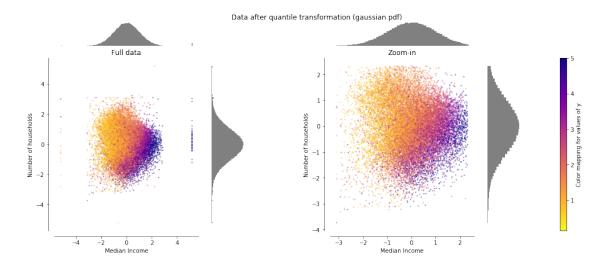
In [19]: make_plot(5)



4.9 QuantileTransformer (Gaussian output)

QuantileTransformer has an additional output_distribution parameter allowing to match a Gaussian distribution instead of a uniform distribution. Note that this non-parameteric transformer introduces saturation artifacts for extreme values.

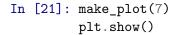
In [20]: make_plot(6)

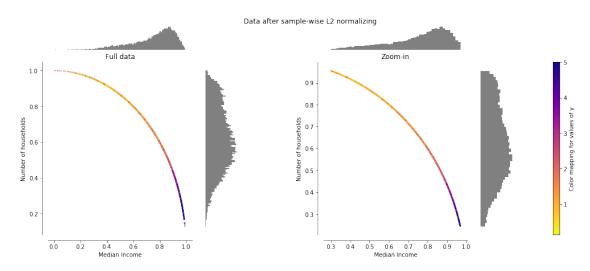


4.10 Normalizer

The Normalizer rescales the vector for each sample to have unit norm, independently of the distribution of the samples. It can be seen on both figures below where all samples are mapped onto the unit circle. In our example the two selected features have only positive values; therefore the

transformed data only lie in the positive quadrant. This would not be the case if some original features had a mix of positive and negative values.





Which scaler should we use?

Let's have a closer look at the robust scaler on our entire dataset:

```
In [22]: df_robust = pd.DataFrame(RobustScaler(quantile_range=(25, 75)).fit_transform(df), col-
         df_robust.head(10)
```

Out[22]:		${\tt MedInc}$	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	\
C)	2.197582	0.631579	1.088935	-0.267221	-0.899787	-0.307981	0.957672	
1	1	2.186664	-0.421053	0.626066	-0.822926	1.316631	-0.830800	0.952381	
2	2	1.707732	1.210526	1.898042	0.263955	-0.714286	-0.018599	0.949735	
3	3	0.967177	1.210526	0.364978	0.259814	-0.648188	-0.316908	0.949735	
4	1	0.142854	1.210526	0.653191	0.345657	-0.640725	-0.746784	0.949735	
5	5	0.230291	1.210526	-0.290055	0.586926	-0.802772	-0.795547	0.949735	
6	3	0.057022	1.210526	-0.184419	-1.042501	-0.076759	-0.809026	0.947090	
7	7 –	0.190288	1.210526	-0.267799	0.139580	-0.009595	-1.208021	0.947090	
8	3 -	0.667202	0.684211	-0.580152	0.736958	0.042644	-0.928102	0.947090	
g	9	0.071748	1.210526	-0.160418	-0.626926	0.410448	-0.757574	0.947090	

Longitude

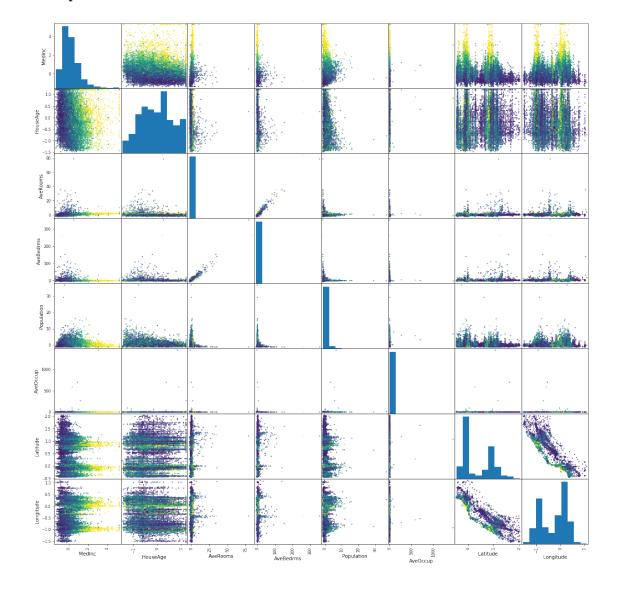
- -0.986807
- -0.984169 1
- 2 -0.989446

-0.992084

3

-0.992084

- 5 -0.992084
- 6 -0.992084
- 7 -0.992084
- 8 -0.994723
- 9 -0.992084



What about the non-linear gaussian transformation, if gaussian distributed shapes are ideal for most machine learning algorithms

In [24]: df_gauss = pd.DataFrame(QuantileTransformer(output_distribution='normal').fit_transformer(output_dis

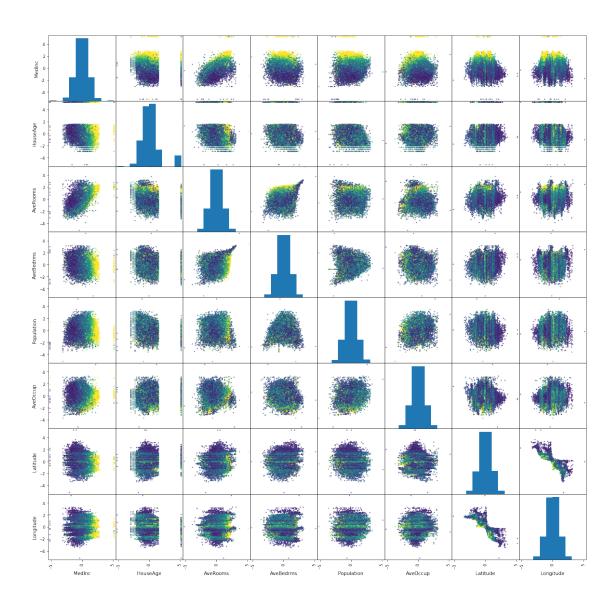
```
0 1.919185 0.912774 1.294622
                                        -0.388543
                                                    -1.697037 -0.450080
                                                                        0.901416
        1 1.914418 -0.479432 0.822470
                                        -1.197835
                                                    1.191955 -1.229273
                                                                        0.886449
        2 1.630171 5.199338
                              1.933184
                                         0.352143
                                                    -1.315958 -0.028306
                                                                       0.879040
        3 1.083447 5.199338
                              0.495717
                                         0.346959
                                                    -1.174755 -0.465169
                                                                        0.879040
        4 0.193151 5.199338 0.852294
                                         0.452858
                                                    -1.164444 -1.109257
                                                                        0.879040
        5 0.298746 5.199338 -0.399051
                                         0.720089
                                                    -1.492879 -1.181873
                                                                        0.879040
        6 0.084155 5.199338 -0.255539
                                                    -0.111890 -1.200185 0.871679
                                        -1.487964
        7 -0.270671 5.199338 -0.367135
                                         0.197601
                                                   -0.015055 -1.812916 0.871679
        8 -1.103892 0.975466 -0.813664
                                         0.861849
                                                   0.060256 -1.361386
                                                                       0.871679
        9 0.107135 5.199338 -0.220709 -0.923979
                                                   0.493081 -1.126478 0.871679
           Longitude
        0 -1.152175
        1 -1.137677
        2 -1.169401
        3 -1.189522
        4 -1.189522
        5 -1.189522
        6 -1.189522
        7 -1.189522
        8 -1.225943
        9 -1.189522
In [25]: scatter_matrix(df_gauss, c=housing.target, alpha=0.8, figsize=(20, 20), s=20)
        plt.show()
```

AveBedrms

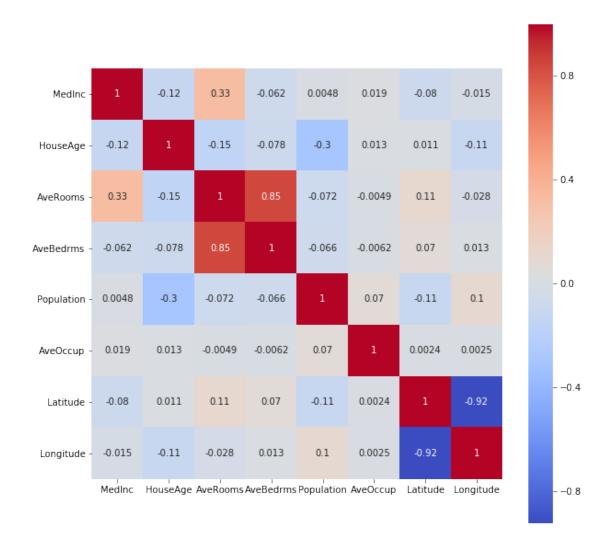
Population AveOccup Latitude \

MedInc HouseAge AveRooms

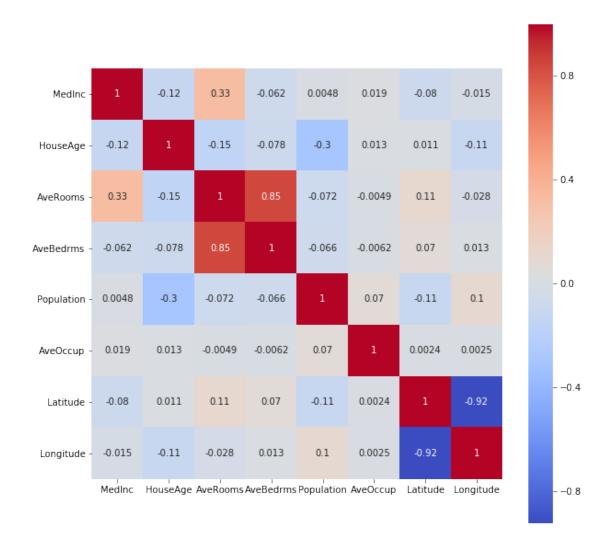
Out [24]:



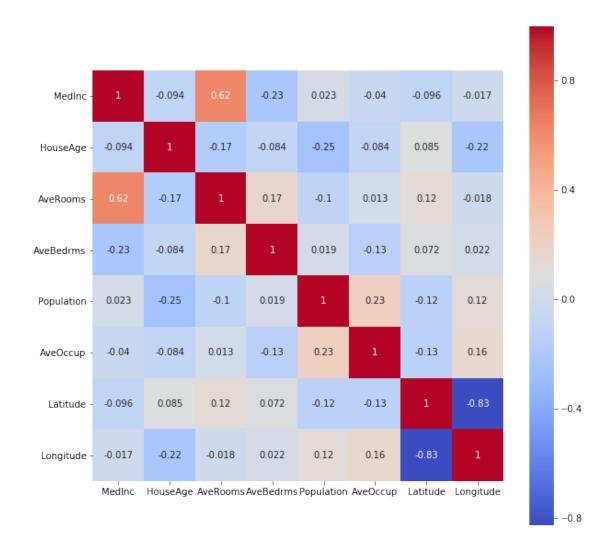
4.12 Impact on the correlations



Out[27]: <matplotlib.axes._subplots.AxesSubplot at 0x7fe8c6620250>



Out[28]: <matplotlib.axes._subplots.AxesSubplot at 0x7fe8c69fd190>



Non-linear transformations smooth out distributions and are less influenced by outliers. However, they distort correlations and distances within and across features. There is no general answer, which scaler will work best for the problem. Like many things in machine learning, this is simply something one need to test/study.

5 A DNN for regression

5.0.1 Task 2: Design a DNN for this regression problem

- Prepare the data by creating a robust scaled design matrix and a minmax scaled target vector and split into training (70%) and test sample.
- Design a simple fully-connected DNN for regression with 4 hidden layers. Use 30% of the training data for validation. Use adam as optimizer and set the batch size to 256.
- What is a good activation function for the output node? What is a good loss function?
- Train the DNN over 300 epochs and plot the loss function and one additional metric for linear regression as a function of epochs.

- Evaluate the obtained model on the testing data, compare the prediction to the true value.
- Use scikit-learn metrics for regression to evaluate the model
- Which feature has the highest linear correlation to the prediction? Plot the true value and the prediction dependent on this feature.

```
In [29]: from sklearn.model_selection import train_test_split
       X_train, X_test, y_train, y_test = train_test_split(df.values, housing.target, test_s
In [30]: y_train
Out[30]: array([1.938, 1.697, 2.598, ..., 2.221, 2.835, 3.25])
In [31]: scaler = RobustScaler(quantile_range=(25, 75))
       X_train = scaler.fit_transform(X_train)
       X_test = scaler.transform(X_test)
       scaler_y = MinMaxScaler()
       y_train = scaler_y.fit_transform(y_train.reshape(-1, 1)).reshape(-1)
       y_test = scaler_y.transform(y_test.reshape(-1, 1)).reshape(-1)
       y_train
Out[31]: array([0.36866034, 0.31896982, 0.50474225, ..., 0.42701061, 0.55360803,
             0.63917468])
In [33]: from keras.models import Sequential
       from keras.layers import Dense
       model = Sequential()
       model.add(Dense(units=128, activation='relu', input_dim=8))
       model.add(Dense(units=64, activation='relu'))
       model.add(Dense(units=32, activation='relu'))
       model.add(Dense(units=8 , activation='relu'))
       model.add(Dense(units=1, activation='sigmoid'))
       model.compile(loss='mse', optimizer='adam', metrics=['mae'])
In [34]: model.summary()
   -----
Layer (type)
             Output Shape
                                             Param #
_____
                       (None, 128)
dense_6 (Dense)
                                             1152
._____
dense_7 (Dense)
                       (None, 64)
                                             8256
               (None, 32)
dense_8 (Dense)
                                              2080
dense_9 (Dense)
                       (None, 8)
                                             264
dense_10 (Dense) (None, 1) 9
```

Total params: 11,761 Trainable params: 11,761 Non-trainable params: 0

5.0.2 Training

```
In [35]: # fix random seed for reproducibility
           seed = 42
           np.random.seed(seed)
           history = model.fit(X_train, y_train, validation_split=0.3, epochs=300, batch_size=25
WARNING:tensorflow:From /home/nackenho/miniconda/envs/TUDortmundMLSeminar/lib/python2.7/site-page warning-page warning-pag
Instructions for updating:
Use tf.cast instead.
Train on 10113 samples, validate on 4335 samples
Epoch 1/300
Epoch 2/300
Epoch 3/300
Epoch 4/300
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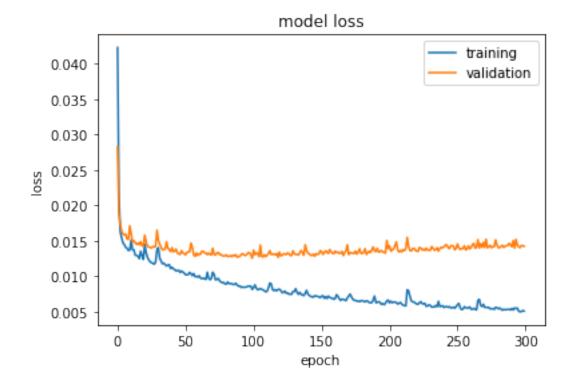
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```

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

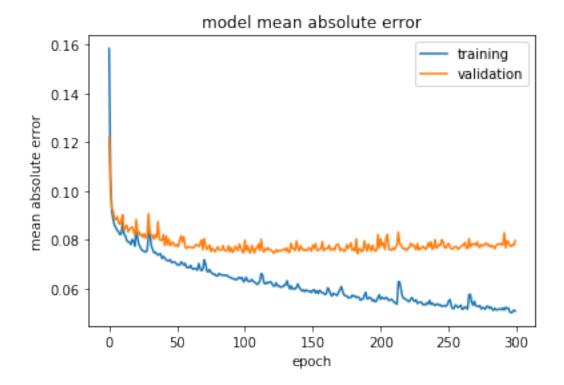
```
In [36]: print(history.history.keys())
```

```
['val_mean_absolute_error', 'loss', 'mean_absolute_error', 'val_loss']
```

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



Similarly, we can plot the mean absolute error



5.0.3 Evaluation

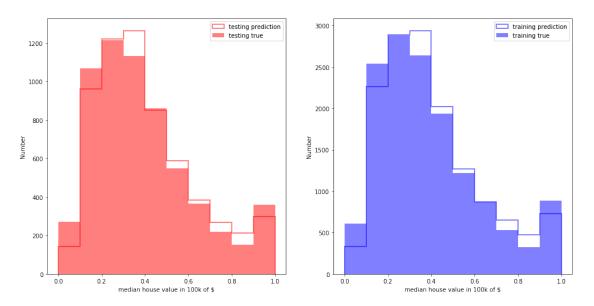
Let's evaluate the loss and mean absolute error on our test data:

Let's make the prediction for our test data:

In order to compare the test prediction with the training prediction, we will also obtain a training prediction:

```
In [42]: y_train_pred = model.predict(X_train, verbose = True, batch_size=256)
        y_train_pred = y_train_pred.reshape(-1)
In [43]: plt.figure(figsize=(16,8))
        plt.subplot(121)
        plt.hist(y_test, alpha=0.5, color='red', range=[0, 1], bins=10)
        plt.hist(y_pred, alpha=0.5, color='red', range=[0, 1], bins=10, histtype='step', line
        plt.xlabel('median house value in 100k of $')
        plt.ylabel('Number')
        plt.legend(['testing prediction', 'testing true'], loc='upper right')
        plt.subplot(122)
        plt.hist(y_train, alpha=0.5, color='blue', range=[0, 1], bins=10)
        plt.hist(y_train_pred, alpha=0.5, color='blue', range=[0, 1], bins=10, histtype='step
        plt.xlabel('median house value in 100k of $')
        plt.ylabel('Number')
        plt.legend(['training prediction', 'training true'], loc='upper right')
```

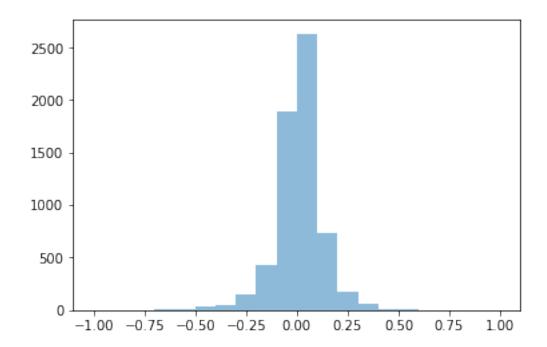
Out[43]: <matplotlib.legend.Legend at 0x7fe84c70ad90>



How well do the histograms agree? We can use the Kolmogorov-Smirnov statistic to quantify that:

```
('Testing KS:', Ks_2sampResult(statistic=0.046834625322997425, pvalue=2.3797666210091484e-06))
('Training KS:', Ks_2sampResult(statistic=0.049210963455149526, pvalue=1.153721091524153e-15))
```

Alternatively, we could also look at the difference between the true and prediction values in order to see the spread on example basis:



5.0.4 Use the scikit learn metrics to evaluate the model

```
In [46]: from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error

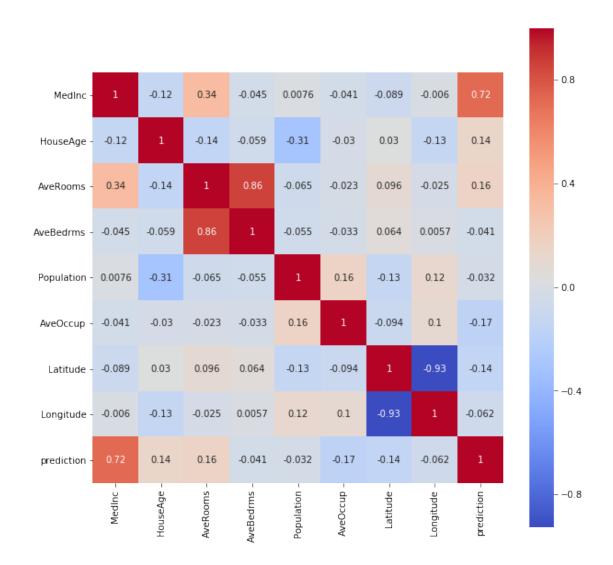
# Explained variance score: 1 is perfect prediction
print('Coefficient of determination: %.2f' % r2_score(y_test, y_pred))
# The mean squared error
print("Mean squared error: %.2f" % mean_squared_error(y_test, y_pred))
# The mean squared error
print("Mean absolute error: %.2f" % mean_absolute_error(y_test, y_pred))
```

Coefficient of determination: 0.75

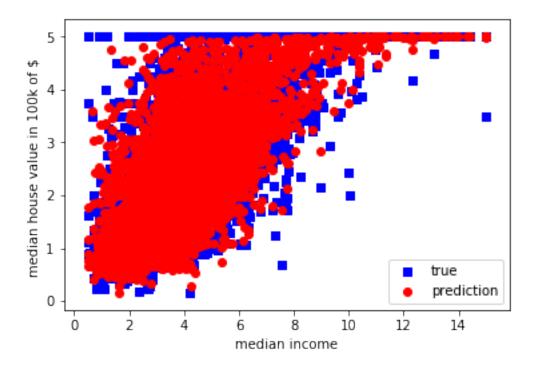
Mean squared error: 0.01 Mean absolute error: 0.08

5.0.5 Plot the correlations of the input features to the predictions

```
In [47]: df out = pd.DataFrame(X test, columns=housing.feature names)
In [48]: df_out.head()
Out [48]:
             MedInc HouseAge AveRooms
                                                   Population AveOccup Latitude \
                                        AveBedrms
        0 -0.848027 -0.210526 -0.645394
                                        -0.290855
                                                     0.239316 1.249230
                                                                        0.473545
        1 -0.460004 0.052632 -0.119769
                                         1.539384
                                                     0.424145 -0.161828 0.230159
        2 -0.026930 1.210526 -0.778816
                                         1.457971
                                                     0.151709 -1.716414 0.933862
        3 1.003492 -0.631579 0.577761 -0.313113
                                                     0.573718 0.739080 0.002646
        4 0.084853 0.263158 0.161667 -0.229352
                                                    -0.112179 -0.392931 0.621693
           Longitude
        0 -0.131926
        1 - 0.250660
        2 -1.036939
        3 -0.055409
        4 -0.902375
In [50]: df_out = df_out.assign(prediction=y_pred)
        df_out.head()
Out [50]:
             MedInc HouseAge AveRooms AveBedrms
                                                   Population AveOccup Latitude \
        0 -0.848027 -0.210526 -0.645394 -0.290855
                                                     0.239316 1.249230 0.473545
        1 -0.460004 0.052632 -0.119769
                                        1.539384
                                                     0.424145 -0.161828 0.230159
        2 -0.026930 1.210526 -0.778816
                                         1.457971
                                                     0.151709 -1.716414 0.933862
        3 1.003492 -0.631579 0.577761
                                       -0.313113
                                                     0.573718 0.739080 0.002646
        4 0.084853 0.263158 0.161667
                                       -0.229352
                                                  -0.112179 -0.392931 0.621693
           Longitude prediction
        0 -0.131926
                        0.073883
        1 -0.250660
                        0.183882
        2 -1.036939
                        0.988333
        3 -0.055409
                        0.545298
        4 -0.902375
                        0.570213
In [51]: plt.figure(figsize=(10,10))
        sns.heatmap(df out.corr(), annot=True, square=True, cmap='coolwarm')
Out[51]: <matplotlib.axes._subplots.AxesSubplot at 0x7fe86c300810>
```



5.0.6 Plot the most important input feature dependent on the true value and the prediction



6 Regularization

The training and validation loss function diverge during the training resulting in a considerably higher validation loss than the data. Can we use regularizer in order to control that?

6.1 L1/L2 Regularizer

6.1.1 Task 3: Train and evaluate the same DNN with an L2 Regularizer

scaler_y = MinMaxScaler(feature_range=(0, 1))

- The regularizer can be simply set by importing from keras.regularizers import 12 and adding kernel_regularizer=12(12_lambda) as option to the Dense layer
- Choose l2_lambda=0.0001
- Perform the same scaling of the inputs
- How does the loss function evolution change?
- How does the performance and the prediction change?

```
In [53]: from sklearn.model_selection import train_test_split
    X_train, X_test, y_train, y_test = train_test_split(df.as_matrix(), housing.target, to
    scaler = RobustScaler(quantile_range=(25, 75))
    X_train = scaler.fit_transform(X_train)
    X_test = scaler.transform(X_test)
```

```
/home/nackenho/miniconda/envs/TUDortmundMLSeminar/lib/python2.7/site-packages/ipykernel_launche
Out[53]: array([0.36866034, 0.31896982, 0.50474225, ..., 0.42701061, 0.55360803,
            0.63917468])
In [55]: from keras.regularizers import 12
      model = Sequential()
      12_{\text{lambda}} = 0.0001
      model.add(Dense(units=128, activation='relu', kernel_regularizer=12(12_lambda), input
      model.add(Dense(units=64, activation='relu', kernel_regularizer=12(12_lambda)))
      model.add(Dense(units=32, activation='relu', kernel_regularizer=12(12_lambda)))
      model.add(Dense(units=8 , activation='relu', kernel_regularizer=12(12_lambda)))
      model.add(Dense(units=1, activation='sigmoid'))
      model.compile(loss='mse', optimizer='adam', metrics=['mae'])
      model.summary()
                    Output Shape
Layer (type)
______
dense_16 (Dense)
                     (None, 128)
                                         1152
dense_17 (Dense)
                     (None, 64)
                                         8256
                    (None, 32)
dense_18 (Dense)
                                         2080
dense 19 (Dense)
                    (None, 8)
                                         264
-----
dense 20 (Dense)
              (None, 1)
______
Total params: 11,761
Trainable params: 11,761
Non-trainable params: 0
In [56]: history = model.fit(X_train, y_train, validation_split=0.3, epochs=300, batch_size=25
Train on 10113 samples, validate on 4335 samples
Epoch 1/300
Epoch 2/300
Epoch 3/300
```

y_train = scaler_y.fit_transform(y_train.reshape(-1, 1)).reshape(-1)

y_test = scaler_y.transform(y_test.reshape(-1, 1)).reshape(-1)

y_train

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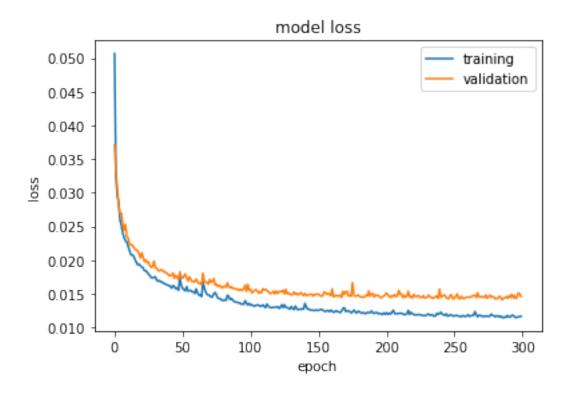
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In [57]: # summarize history for loss
  plt.plot(history.history['loss'])
  plt.plot(history.history['val_loss'])
  plt.title('model loss')
  plt.ylabel('loss')
  plt.xlabel('epoch')
```

plt.legend(['training', 'validation'], loc='upper right')

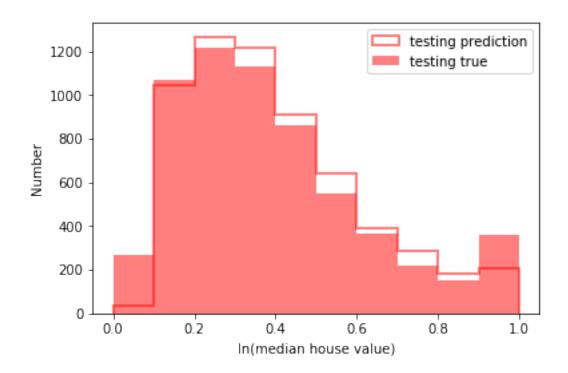
plt.show()



```
In [58]: loss_and_metrics = model.evaluate(X_test, y_test, batch_size=256)
        print loss_and_metrics
        y_pred = model.predict(X_test, verbose = True, batch_size=256)
=======] - Os 18us/step
[0.013912828256513259, 0.07427210252953438]
6192/6192 [=========] - Os 46us/step
In [59]: # Explained variance score: 1 is perfect prediction
        print('Coefficient of determination: %.2f' % r2_score(y_test, y_pred))
        # The mean squared error
        print("Mean squared error: %.2f" % mean_squared_error(y_test, y_pred))
        # The mean squared error
        print("Mean absolute error: %.2f" % mean_absolute_error(y_test, y_pred))
Coefficient of determination: 0.79
Mean squared error: 0.01
Mean absolute error: 0.07
In [60]: # predictions
        y_pred.reshape(-1)
```

```
plt.hist(y_test, alpha=0.5, color='red', range=[0, 1], bins=10)
plt.hist(y_pred, alpha=0.5, color='red', range=[0, 1], bins=10, histtype='step', line
plt.xlabel('ln(median house value)')
plt.ylabel('Number')
plt.legend(['testing prediction', 'testing true'], loc='upper right')
```

Out[60]: <matplotlib.legend.Legend at 0x7fe82c6c32d0>



6.2 Dropout

```
In [61]: from sklearn.model_selection import train_test_split
    X_train, X_test, y_train, y_test = train_test_split(df.as_matrix(), housing.target, to
    scaler = RobustScaler(quantile_range=(25, 75))
    X_train = scaler.fit_transform(X_train)
    X_test = scaler.transform(X_test)

scaler_y = MinMaxScaler()
    y_train = scaler_y.fit_transform(y_train.reshape(-1, 1)).reshape(-1)
    y_test = scaler_y.transform(y_test.reshape(-1, 1)).reshape(-1)
    y_train
```

/home/nackenho/miniconda/envs/TUDortmundMLSeminar/lib/python2.7/site-packages/ipykernel_launche

```
Out[61]: array([0.36866034, 0.31896982, 0.50474225, ..., 0.42701061, 0.55360803,
                                0.63917468])
In [62]: from keras.layers import Dropout
                  model = Sequential()
                  dropout=0.2
                  model.add(Dense(units=128, activation='relu', input_dim=8))
                  model.add(Dropout(dropout))
                  model.add(Dense(units=64, activation='relu'))
                  model.add(Dropout(dropout))
                  model.add(Dense(units=32, activation='relu'))
                  model.add(Dropout(dropout))
                  model.add(Dense(units=8 , activation='relu'))
                  model.add(Dropout(dropout))
                  model.add(Dense(units=1, activation='sigmoid'))
                  model.compile(loss='mse', optimizer='adam', metrics=['mae'])
                  model.summary()
WARNING:tensorflow:From /home/nackenho/miniconda/envs/TUDortmundMLSeminar/lib/python2.7/site-page warning-page warning-pag
Instructions for updating:
Please use `rate` instead of `keep_prob`. Rate should be set to `rate = 1 - keep_prob`.
Layer (type) Output Shape
                                                                                                            Param #
______
                                                       (None, 128)
dense_21 (Dense)
                                                                                                             1152
dropout_1 (Dropout)
                                                       (None, 128)
dense_22 (Dense) (None, 64)
                                                                                          8256
dropout_2 (Dropout)
                                            (None, 64)
                                         (None, 32)
dense_23 (Dense)
                                                                                                             2080
                                            (None, 32)
dropout_3 (Dropout)
 -----
dense_24 (Dense)
                                                       (None, 8)
                                                                                                             264
                                            (None, 8)
dropout_4 (Dropout)
 -----
dense_25 (Dense) (None, 1)
______
Total params: 11,761
Trainable params: 11,761
Non-trainable params: 0
```

In [63]: history = model.fit(X_train, y_train, validation_split=0.3, epochs=300, batch_size=25

```
Train on 10113 samples, validate on 4335 samples
Epoch 1/300
Epoch 2/300
Epoch 3/300
Epoch 4/300
Epoch 5/300
Epoch 6/300
Epoch 7/300
Epoch 8/300
Epoch 9/300
Epoch 10/300
Epoch 11/300
Epoch 12/300
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Epoch 24/300
```

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Epoch 25/300
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```

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Epoch 239/300
Epoch 240/300
```

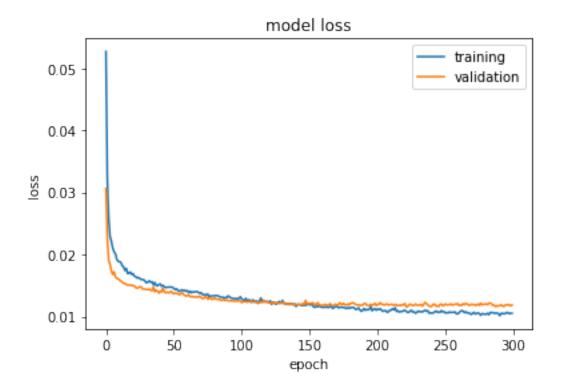
```
Epoch 241/300
Epoch 242/300
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Epoch 299/300
Epoch 300/300
In [64]: # summarize history for loss
 plt.plot(history.history['loss'])
 plt.plot(history.history['val_loss'])
 plt.title('model loss')
 plt.ylabel('loss')
 plt.xlabel('epoch')
```

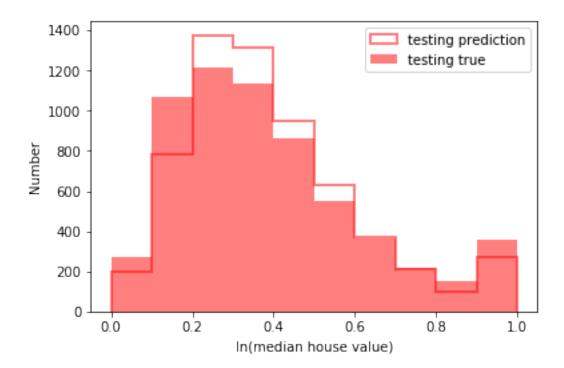
plt.legend(['training', 'validation'], loc='upper right')

plt.show()



You have to treat this result with care: The training loss is evaluated after each batch, where nodes are dropped, while the validation loss is calculated after one epoch, where all nodes are included.

Out[67]: <matplotlib.legend.Legend at 0x7fe816e26950>



6.3 Task 4 (Bonus) - Playtime

- What do you need to change in the DNN if you don't scale the target vector?
- How does the result change if you use a quantile transformer with uniform output?
- How does the L1 regularizer perform?
- What happens if you change the L2 regularizer strength?
- What happens if you change the drop out percentage?
- How does the result change if you use only the 3 most important features?