# Notes to Models

This section describes the statistical models that we used to predict apartment prices based on their feature set. The goal is to contruct different models of varying complexity and compare both their in-sample and their out-of-sample performance on the Airbnb data.

At this point in the data pipeline all preprocessing steps are completed such that all covariates have the correct data type to be used by the models. Whereas the selected classical Machine Learning models described in section 1 use input features as numpy arrays, the Neural Network in section 2 first converts them to *Tensors*, the canonical data type across all popular Deep Learning Frameworks.

# 1 Classical Models

- serve as benchmark models to better evaluate performance of custom neural network
- selected with increasing degrees of complexity and corresponding decreasing degree of interpretability
- Focus on 4 models: LinearRegression, Ridge, RandomForest and HistGradientBoosting
- Describe Model Fitting process and hyperparameter tuning with Randomized Search Cross Validation

## 2 Neural Network

#### 2.1 Architecture

The network's design is restricted by two factors:

- 1. The number of input features in the *first* layer has to equal the number of features used for prediction.
- 2. The number of output features in the *last* layer is fixed to 1 since the network directly predicts the price as a scalar quantity.

All intermediary layers and thus both the *width* and the *depth* of the network are free to choose. After experimenting with many different configurations, mostly inspired by empirical findings in the literature, we finally settled with a fairly simple *block structure*.

Starting from roughly 60 input features, the network width is first blown up to 256 features before steadily decreasing it again to a single output neuron in the final layer. More precisely, the architecture consists of 6 intermediary blocks with 64, 128, 256, 128, 64 and 8 output features in addition to the linear input and output layers.

The structure of each so-called Linear Block is displayed in figure 1. We now explain the reasoning behind including or excluding elements in this configuration.

## Linear Layer

Each Linear Block is based on a four-element cycle that is repeated twice. Each cycle starts with a Fully-Connected Layer containing the majority of trainable weights in the network. The first linear layer determines the output dimension of this block, in our case mostly doubling or halving the number of input features. Since both linear layers are immediately followed by a Batchnorm Layer, the additional Bias term is redundant and thus omitted.

#### Batchnorm

Batchnorm Layers often lead to a more well-behaved training process. By means of first standardizing the activations within each minibatch and rescaling them afterwards, the network *learns* a convenient magnitude of the activations. This tends to be particularly effective for *saturating* activation functions such as sigmoid or tanh activations, positive effects for training,

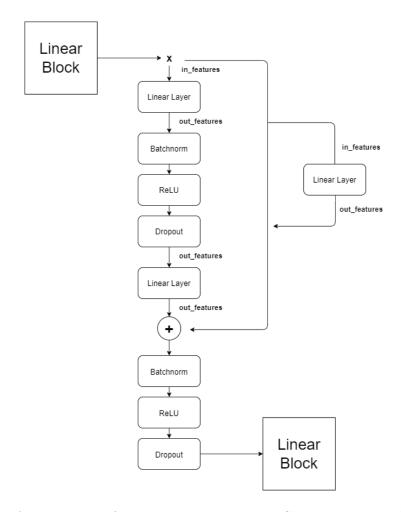


Figure 1: Architecture of each Block in the Fully Connected Neural Network

however, have also been observed for the ReLU activation function, which is used in our design. Of all individual components of the Linear Block structure, Batchnorm was the least important and provided only marginal benefits.

#### ReLU

Out of the numerous options for including nonlinearities into the network and thus expanding the function space that the network is able to learn, we settled for the default choice of the *Rectified Linear Unit* activation. While briefly experimenting with the related Leaky ReLU and Exponential ReLU,

the differences were insignificant and could be easily attributed to other factors such as random weight initialization.

### **Dropout**

The Dropout Layer at the end of each cycle turned out to be the single most impactful factor for the network's generalization ability. In fact, due to the different behaviour of dropout during training and inference, we could directly control the relative performance on training and validation set by varying the dropout probability p.

More specifically, the network overfitted drastically by setting p to zero. This actually provided the valuable insight that the current function class is flexible enough to model the task at hand properly. Thus, there was no need to artificially expand the network size beyond the current quite compact architecture with roughly 280.000 trainable parameters, saving computation time as a nice side-effect.

Figure 2 displays the shift in performance metrics on training and validation set when steadily increasing the dropout probability p. While not beneficial for overall performance, dropout delivers a leverage to make the model perform much better on out-of-sample data compared to the dataset that it was actually trained on.

This behaviour can be explained by the *ensemble* interpretation of dropout: In each epoch, a different subset of neurons is excluded to contribute to training and thus a distinct subset model, nested in the full model, is responsible for the prediction output. If the dropout probability is extremely high, these subset models are simply too different from each other and do *not agree* on a common range of sensible prediction values.

In contrast, during inference (and possible deployment of the model), any randomness should be avoided and the network may use all of its neurons. Although there is no influence on the model weights in this stage, the model pools all subset models together and averages out the diverging effects of each component, ultimately resulting in better performance metrics.

### **Residual Connections**

One special feature of the Linear Block architecture in 1 is the *Residual Connection* adding the block input to the output of the second linear layer within each block. This component was originally implemented having a fairly deep network in mind since *Residual Blocks* introduced by the famous

ResNet architecture are a very popular tool for stable gradient flow by preventing the issue of vanishing gradients.

As mentioned above the actual depth of the final model turned out to be limited. Therefore we decided to enable inclusion and exclusion of skip-connections in the network by a boolean parameter allowing for easy comparisons between the model designs. Although the residual component did not have a major impact on performance, it was slightly beneficial in most settings such that there was no reason to remove it from the architecture.

There are two aspects worth mentioning about the residual connection in figure 1:

- 1. The addition of the input with the output of the second linear layer is performed **before** the final Batchnorm and ReLU layers of this block. This guarantees a nonnegative input in the expected range for the next Linear Block since the raw outputs of a fully connected layer are (in theory) unbounded.
- 2. One caveat of the residual architecture is to ensure that at addition time all contributing terms share the same dimensions. In case of a fully connected layer dealing with two-dimensional tensors, this amounts to an equal number of features in the second dimension. As illustrated by the annotations in figure 1, this restriction requires an extra step if the number of input features is different from the number of output features in this particular block. In our case the dimnesions adjustment is performed by an additional linear layer exclusively for the block input x.

# 2.2 Further (Hyper)-Parameters

## Optimizer and Weight Decay

Similar to ReLU as the default activation function Adam has evolved to the default choice for performing the optimisation step when training the neural network. Indeed, the loss curves during the training process looked much smoother when using Adam instead of vanilla Gradient Descent. Additionally, there was no need for introducing a *penalty term* on the weights of the network while using Adam, whereas Gradient Descent (with optional Momentum) did benefit slightly from a  $L_2$ -Penalty.

Moreover, we did not make use of other penalty implementations such as a  $L_1$  penalty which can often induce sparseness into the model. On the one hand adding neither the  $L_1$ - nor the  $L_2$ -Norm of the weights to the loss function showed promising improvements in performance, on the other hand, for interpretability reasons, we preferred to induce 'sparseness' explicitly by manual and automatic feature selection prior to the model training itself rather than relying on implicit effects inside of the network 'black box'.

#### Loss Function

Since we are in a Regression context for predicting the continuous price variable, we chose the standard Mean Squared Errro loss function. This has the additional nice property that, in case of a normal distribution with constant variance, i.e. price  $\sim \mathcal{N}(\mu, \sigma^2)$ , the model minimizing the MSE-Loss simultaneously maximizes the Gaussian Likelihood, providing a probabilistic interpretation.

## Learning Rate

Throughout training the network with different configurations of hyperparameters we kept the learning rate fixed at 0.01. Since using a larger learning rate at early stages of training did indeed show promising effects, we experimented with different learning rate *schedulers*, either decreasing the learning rate in fixed intervals by a constant or exponential rate or decreasing the learning rate whenever the loss seems to stagnate for some given window.

However, the benefits of faster loss decay at the beginning of training was overweighed by the difficulties of too small learning rates at later stages in the training loop. All settings we tried introduced a too aggressive learning rate in flatter regions of the loss surface whereas a constant learning rate still lead to a steady loss decrease.

Moreover, since computation time was not too expensive due to the compact network size, we could easily make up for the slower initial progress with a fixed learning rate by simply training the model for more epochs (typically around 200 where the model weights were saved at the point of best performance on the validation set), ultimately leading to a lower training and validation loss.

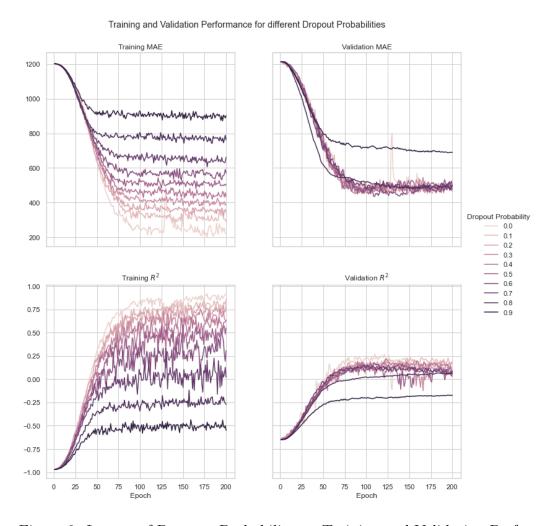


Figure 2: Impact of Dropout Probability on Training and Validation Performance