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| --- | --- |
| **Hyperparameter** | **Meaning** |
| batch\_size | <https://www.tensorflow.org/api_docs/python/tf/keras/Model>  Integer or None. Number of samples per gradient update. If unspecified, batch\_size will default to 32. Do not specify the batch\_size if your data is in the form of datasets, generators, or [keras.utils.Sequence](https://www.tensorflow.org/api_docs/python/tf/keras/utils/Sequence) instances (since they generate batches). |
| beta\_1 | Used in ANN\_tf2, part of the Adam ANN optimizer  <https://keras.io/api/optimizers/adam/>  beta\_1: A float value or a constant float tensor, or a callable that takes no arguments and returns the actual value to use. The exponential decay rate for the 1st moment estimates. Defaults to 0.9. |
| bypass | Shows up in ANN\_tf2 in nets.py  Has to do with connecting non-adjacent layers in the ANN  Has to do with tf.keras.layers.Concatenate  <https://www.tensorflow.org/api_docs/python/tf/keras/layers/concatenate>  <https://www.tensorflow.org/api_docs/python/tf/keras/layers/Concatenate>  Layer that concatenates a list of inputs. |
| decay | Used in ANN\_tf2 in nets.py, specifically in the Adam ANN optimizer  <http://man.hubwiz.com/docset/TensorFlow.docset/Contents/Resources/Documents/api_docs/python/tf/keras/optimizers/Adam.html>  decay: float >= 0. Learning rate decay over each update. |
| drop\_rate | Used in ANN\_tf2 in nets.py, specifically in tf.keras.layers.Dropout  Dropout helps prevent overfitting  <https://www.tensorflow.org/api_docs/python/tf/keras/layers/Dropout>  Rate: Float between 0 and 1. Fraction of the input units to drop. |
| hidden\_size | Used in ANN\_tf2 in nets.py  How many inner layers there are, and how many nodes in each layer  Dense, BatchNormalization, LeakyReLU, Dropout |
| lr | Used in ANN\_tf2 in nets.py, specifically in the Adam ANN optimizer  <http://man.hubwiz.com/docset/TensorFlow.docset/Contents/Resources/Documents/api_docs/python/tf/keras/optimizers/Adam.html>  Learning rate |
| reg | Used in ANN\_tf2 in nets.py  kernel\_regularizer=tf.keras.regularizers.l2(\*reg used here\*) |
| res | Used in ANN\_tf2 in nets.py  Has to do with tf.keras.layers.Add  <https://www.tensorflow.org/api_docs/python/tf/keras/layers/Add>  Layer that adds a list of inputs. |
| amsgrad | Used in nets.py, with tf.keras.optimizers.Adam  <https://www.tensorflow.org/api_docs/python/tf/keras/optimizers/Adam>  Boolean. Whether to apply AMSGrad variant of this algorithm from the paper "On the Convergence of Adam and beyond". Defaults to False. |
| patience | Used in EarlyStopping in model\_optimization.py  <https://keras.io/api/callbacks/early_stopping/>  Number of epochs with no improvement after which training will be stopped. |
| epochs | <https://www.tensorflow.org/api_docs/python/tf/keras/Model>  Integer. Number of epochs to train the model. An epoch is an iteration over the entire x and y data provided. Note that in conjunction with initial\_epoch,epochs is to be understood as "final epoch". The model is not trained for a number of iterations given by epochs, but merely until the epoch of index epochs is reached. |

Functions calling each other

optimize (optimize\_ann.py)

train\_model\_hyperopt (molSimplifyAD/retrain/model\_optimization.py)

build\_ANN (molSimplifyAD/retrain/nets.py)

ANN\_tf2 (molSimplifyAD/retrain/nets.py)

tf.keras.Model