overfit_and_underfit.ipynb - Colaboratory

▼ Setup

Before getting started, import the necessary packages:.

1 !pip install -q git+https://github.com/tensorflow/docs
2
3 import tensorflow_docs as tfdocs
4 import tensorflow_docs.modeling
5 import tensorflow_docs.plots

Building wheel for tensorflow-docs (setup.py) ... done

```
1 from IPython import display
2 from matplotlib import pyplot as plt
3
4 import numpy as np
5
6 import pathlib
7 import shutil
8 import tempfile
9
```

1 logdir = pathlib.Path(tempfile.mkdtemp())/"tensorboard_logs"
2 shutil.rmtree(logdir, ignore_errors=True)

▼ The Higgs Dataset

The goal of this tutorial is not to do particle physics, so don't dwell on the details of the dataset. It contains 11 000 000 examples, each with 28 features, and a binary class label.

1 gz = tf.keras.utils.get_file('HIGGS.csv.gz', 'https://archive.ics.uci.edu/ml/machine-learning-databases/00280/HIGGS.csv.gz')

1 FEATURES = 28

The tf.data.experimental.CsvDataset class can be used to read csv records directly from a gzip file with no intermediate decompression

1 ds = tf.data.experimental.CsvDataset(gz,[float(),]*(FEATURES+1), compression_type="GZIP")

That csv reader class returns a list of scalars for each record. The following function repacks that list of scalars into a (feature_vector, label)

```
1 def pack_row(*row):
2   label = row[0]
3   features = tf.stack(row[1:],1)
4   return features, label
```

TensorFlow is most efficient when operating on large batches of data.

So instead of repacking each row individually make a new Dataset that takes batches of 10000-examples, applies the pack_row function to each batch, and then splits the batches back up into individual records:

1 packed_ds = ds.batch(10000).map(pack_row).unbatch()

▼ EDA

Have a look at some of the records from this new packed_ds.

The features are not perfectly normalized, but this is sufficient for this tutorial.

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 print(list(ds.take(2).as_numpy_iterator())[0])
4 print(list(ds.take(2).as_numpy_iterator())[1])
```

(1.0, 0.8692932, -0.6350818, 0.22569026, 0.32747006, -0.6899932, 0.75420225, -0.24857314, -1.0920639, 0.0, 1.3749921, -0.6536742, 0.9303491, 1.1074361, 1.1389043, -1.5781983, -1.0469854, 0.0, 0.65792954, -0.01045457, -0.04576717, 3.1019614, 1.35376, 0.9795631, 0.97807616, (1.0, 0.9075421, 0.32914728, 0.32914728, 0.35941187, 1.4979699, -0.31300953, 1.0955306, -0.5575249, -1.5882298, 2.1730762, 0.8125812, -0.21364193, 1.2710146, 2.2148721, 0.49999395, -1.2614318, 0.73215616, 0.0, 0.3987009, -1.1389301, -0.0008191102, 0.0, 0.3022199, 0.83304816, 0.9856996

```
1 featVals=[features.numpy()[0] for features,label in packed_ds.take(1000)]
2
3 t=packed_ds.take(20000)
```

▼ Target Variable

```
1 t = [label.numpy() for features,label in packed_ds.take(20000)]
2 print("Values 1:",sum(t))
3 print("Values 0:",sum(np.equal(t,0)))
4
Values 1: 10457.0
```

▼ Predictors

Values 0: 9543

```
1 t = np.array([features.numpy() for features,label in packed_ds.take(20000)])
2 print("Min Value:",min(t.flatten()))
3 print("Max Value:",max(t.flatten()))

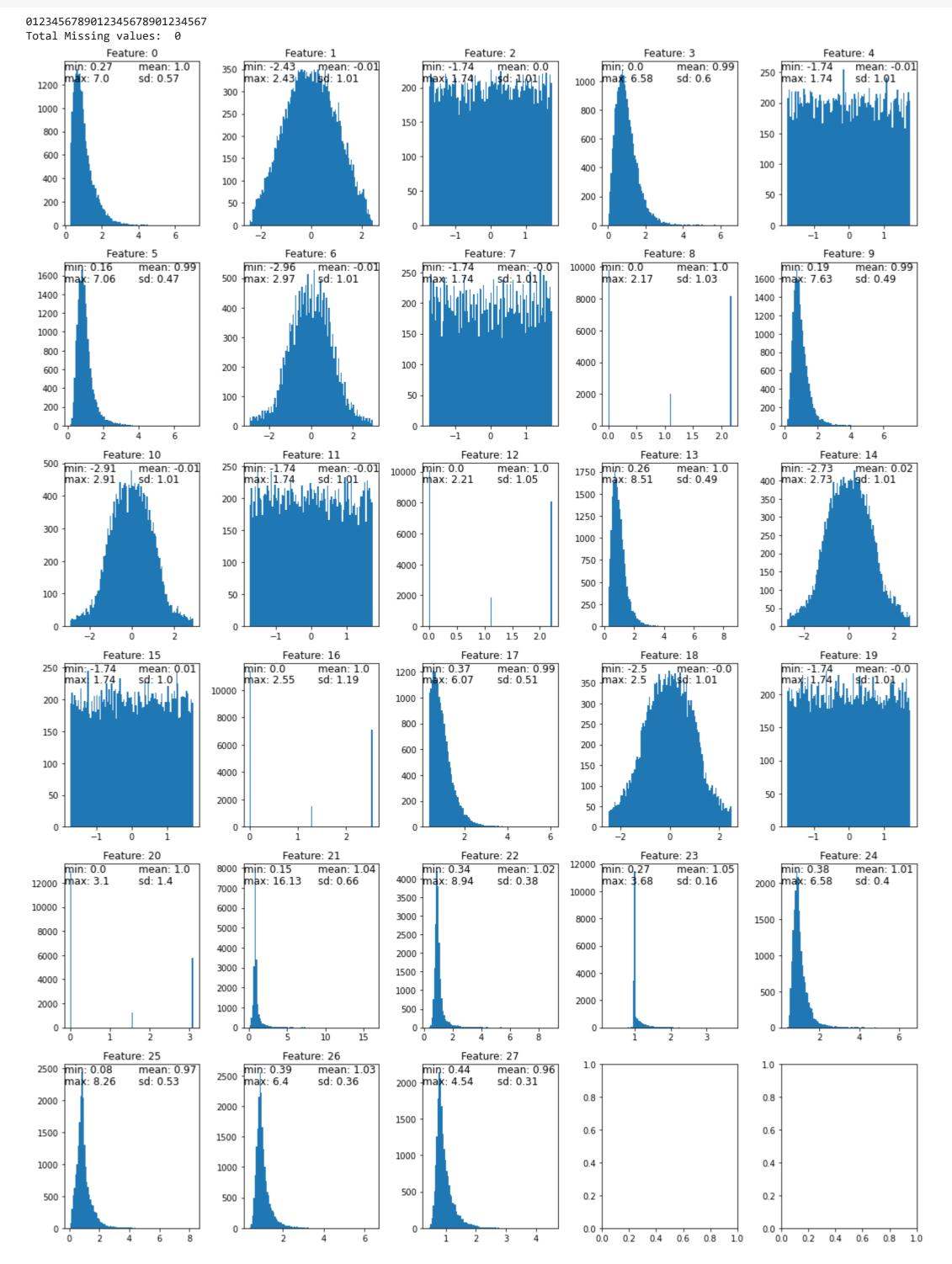
Min Value: -2.960813
Max Value: 16.131908

1 #for features,label in packed_ds.batch(1000).take(1):
```

4 https://colab.research.google.com/github/ngupta23/ds7333_qtw/blob/max%2Fcs6/case_study_6/analysis/master/cs6.ipynb#scrollTo=uXJxtwBWIhjG

2 fig, axs = plt.subplots(6, 5,figsize=(15,20))
3 fig.subplots_adjust(hspace = .2, wspace=.1)

```
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     5 axs = axs.ravel()
     6 totMissing=0
    7 for f in range([len(x) for x in ds.take(1)][0]-1):
     8 print(f % 10,end='')
    9 featVals=[features.numpy()[f] for features,label in packed_ds.take(20000)]
    10 ax=axs[f]
    11 ax.hist(featVals ,bins = 100)
    12 ax.set_title('Feature: ' + str(f))
    ax.text(x=0,y=1,s='min: '+str(round(min(featVals),2)), transform=ax.transAxes, fontsize=12,verticalalignment='top')
    ax.text(x=0,y=0.93,s='max: '+str(round(max(featVals),2)), transform=ax.transAxes, fontsize=12,verticalalignment='top')
    ax.text(x=0.55,y=1,s='mean: '+str(round(np.mean(featVals),2)), transform=ax.transAxes, fontsize=12,verticalalignment='top')
    ax.text(x=0.55,y=0.93,s='sd: '+str(round(np.std(featVals),2)), transform=ax.transAxes, fontsize=12,verticalalignment='top')
    17 totMissing += sum(np.isnan(featVals))
    18 #if(f % 4 !=0):
    19
         #ax.get_yaxis().set_visible(False)
    20 plt.tight_layout()
    21 print("\nTotal Missing values: ", totMissing)
    22
   23
```



Sampling

To keep this tutorial relatively short use just the first 1000 samples for validation, and the next 10 000 for training:

```
1 N_VALIDATION = int(1e3)
2 N_{TRAIN} = int(1e4)
3 BUFFER_SIZE = int(1e4)
4 BATCH_SIZE = 500 # TODO: Note that the paper used 100, we can increase this to reduce training time.
5 STEPS_PER_EPOCH = N_TRAIN//BATCH_SIZE
```

The Dataset.skip and Dataset.take methods make this easy.

At the same time, use the Dataset.cache method to ensure that the loader doesn't need to re-read the data form the file on each epoch:

```
1 validate ds = packed ds.take(N VALIDATION).cache()
2 train_ds = packed_ds.skip(N_VALIDATION).take(N_TRAIN).cache()
1 train_ds
```

<CacheDataset shapes: ((28,), ()), types: (tf.float32, tf.float32)>

These datasets return individual examples. Use the .batch method to create batches of an appropriate size for training. Before batching also remember to .shuffle and .repeat the training set.

```
1 validate_ds = validate_ds.batch(BATCH_SIZE)
2 train_ds = train_ds.shuffle(BUFFER_SIZE).repeat().batch(BATCH_SIZE)
```

Training procedure

1 tf.range(25, dtype=tf.float32)

<tf.Tensor: shape=(25,), dtype=float32, numpy=

Many models train better if you gradually reduce the learning rate during training. Use optimizers.schedules to reduce the learning rate over time:

```
1 # https://www.tensorflow.org/tutorials/text/transformer
 2 class CustomSchedule(tf.keras.optimizers.schedules.LearningRateSchedule):
 3 def __init__(self):
      super(CustomSchedule, self).__init__()
 6 def __call__(self, step):
      ## Original Paper
      # update_callbacks=pylearn2.training_algorithms.sgd.ExponentialDecay(
9
                                           decay_factor=1.0000002, \# Decreases by this factor every batch. (1/(1.000001^8000)^100)
                                           min lr=.000001
10
11
12
      # Implementation in TensorFlow
13
      lr = tf.clip_by_value(0.05 / 1.0000002**step, clip_value_min=0.000001, clip_value_max=0.05)
      return lr
15
16
```

array([0., 1., 2., 3., 4., 5., 6., 7., 8., 9., 10., 11., 12.,

```
https://colab.research.google.com/github/ngupta23/ds7333\_qtw/blob/max\%2Fcs6/case\_study\_6/analysis/master/cs6.ipynb\#scrollTo=uXJxtwBWIhjG
```

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```
13., 14., 15., 16., 17., 18., 19., 20., 21., 22., 23., 24.],
          dtype=float32)>
1 temp_lr_schedule = CustomSchedule()
2 plt.figure(figsize = (8,6))
3 lrs = temp_lr_schedule(tf.range(40000000, dtype=tf.float32))
4 plt.plot(lrs)
5 plt.ylabel("Learning Rate")
6 plt.xlabel("Train Step")
    Text(0.5, 0, 'Train Step')
```

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```
0.05
0.04
0.03
0.02
0.01
0.00
                     1.0
                            1.5
                                            2.5
                                    2.0
```

```
1 lrs
    <tf.Tensor: shape=(40000000,), dtype=float32, numpy=
                    , 0.04999999, 0.04999998, ..., 0.00091578, 0.00091578,
           0.00091578], dtype=float32)>
1 def get_optimizer():
2 lr_schedule = CustomSchedule()
```

Each model in this tutorial will use the same training configuration. So set these up in a reusable way, starting with the list of callbacks.

The training for this tutorial runs for many short epochs. To reduce the logging noise use the tfdocs. EpochDots which simply a . for each epoch and, and a full set of metrics every 100 epochs.

Next include callbacks. EarlyStopping to avoid long and unnecessary training times. Note that this callback is set to monitor the

val_binary_crossentropy, not the val_loss. This difference will be important later.

Use callbacks. TensorBoard to generate TensorBoard logs for the training.

3 return tf.keras.optimizers.SGD(lr_schedule, momentum=0.9)

```
1 def get_callbacks(name):
2 return [
     tfdocs.modeling.EpochDots(),
     tf.keras.callbacks.EarlyStopping(monitor='val_binary_crossentropy', min_delta=0.00001, patience=10),
     tf.keras.callbacks.TensorBoard(logdir/name),
6
```

Similarly each model will use the same Model.compile and Model.fit settings:

```
1 def compile_and_fit(model, name, optimizer=None, max_epochs=10000):
 2 if optimizer is None:
     optimizer = get_optimizer()
    model.compile(optimizer=optimizer,
                  loss=tf.keras.losses.BinaryCrossentropy(from_logits=True),
                  # loss=tf.keras.metrics.AUC(),
 6
 7
                  metrics=[
 8
                    tf.keras.metrics.AUC(name='AUC'),
                    tf.keras.losses.BinaryCrossentropy(from_logits=True, name='binary_crossentropy'),
 9
10
11
12 model.summary()
13
14 history = model.fit(
15
      train_ds,
      steps_per_epoch = STEPS_PER_EPOCH,
17
      epochs=max_epochs,
18
      validation_data=validate_ds,
      callbacks=get_callbacks(name),
20
      verbose=2)
21 return history
```

Model from Paper

1 size_histories = {}

```
1 # https://www.tensorflow.org/api_docs/python/tf/keras/initializers/RandomNormal
 2 first_initializer = tf.keras.initializers.RandomNormal(mean=0., stddev=0.1, seed=42)
 3 outer_initializer = tf.keras.initializers.RandomNormal(mean=0., stddev=0.001, seed=42)
 4 other_initializers = tf.keras.initializers.RandomNormal(mean=0., stddev=0.05, seed=42)
 6 # Top Layer (https://www.quora.com/Are-the-top-layers-of-a-deep-neural-network-the-first-layers-or-the-last-layers)
 7 # Weight Decay: https://machinelearningmastery.com/how-to-reduce-overfitting-in-deep-learning-with-weight-regularization/
 8 weight_decay=0.00001
 9 paper_model = tf.keras.Sequential([
      layers.Dense(300, activation='tanh', input_shape=(FEATURES,), kernel_initializer=first_initializer, kernel_regularizer=12(weight_decay)),
      layers.Dense(300, activation='tanh', kernel_initializer=other_initializers, kernel_regularizer=12(weight_decay)),
      layers.Dense(300, activation='tanh', kernel_initializer=other_initializers, kernel_regularizer=12(weight_decay)),
      layers.Dense(300, activation='tanh', kernel_initializer=other_initializers, kernel_regularizer=12(weight_decay)),
13
      layers.Dropout(0.5), # Top Hidden Layer
      layers.Dense(1, activation='sigmoid', kernel_initializer=outer_initializer, kernel_regularizer=12(weight_decay))
15
16
17 ])
```

```
1 size_histories['paper'] = compile_and_fit(paper_model, 'sizes/paper')
```

https://colab.research.google.com/github/ngupta23/ds7333_qtw/blob/max%2Fcs6/case_study_6/analysis/master/cs6.ipynb#scrollTo=uXJxtwBWIhjG

```
.20/20 - 0s - loss: 0.6694 - AUC: 0.6677 - binary_crossentropy: 0.6618 - accuracy: 0.5994 - val_loss: 0.6729 - val_AUC: 0.6504 - val_binary_crossentropy: 0.6653 - val_accuracy: 0.5570
Epoch 34/10000
.20/20 - 0s - loss: 0.6696 - AUC: 0.6665 - binary_crossentropy: 0.6621 - accuracy: 0.5970 - val_loss: 0.6716 - val_AUC: 0.6622 - val_binary_crossentropy: 0.6640 - val_accuracy: 0.5530
Epoch 35/10000
.20/20 - 0s - loss: 0.6683 - AUC: 0.6723 - binary_crossentropy: 0.6607 - accuracy: 0.5988 - val_loss: 0.6716 - val_AUC: 0.6555 - val_binary_crossentropy: 0.6640 - val_accuracy: 0.5680
Epoch 36/10000
.20/20 - 0s - loss: 0.6689 - AUC: 0.6715 - binary_crossentropy: 0.6613 - accuracy: 0.5972 - val_loss: 0.6711 - val_AUC: 0.6611 - val_binary_crossentropy: 0.6636 - val_accuracy: 0.5580
Epoch 37/10000
.20/20 - 0s - loss: 0.6674 - AUC: 0.6768 - binary crossentropy: 0.6598 - accuracy: 0.5983 - val loss: 0.6706 - val AUC: 0.6664 - val binary crossentropy: 0.6630 - val accuracy: 0.5980
Epoch 38/10000
.20/20 - 0s - loss: 0.6675 - AUC: 0.6785 - binary crossentropy: 0.6599 - accuracy: 0.6094 - val loss: 0.6713 - val AUC: 0.6641 - val binary crossentropy: 0.6638 - val accuracy: 0.5560
Epoch 39/10000
.20/20 - 0s - loss: 0.6681 - AUC: 0.6747 - binary crossentropy: 0.6605 - accuracy: 0.6014 - val loss: 0.6692 - val AUC: 0.6707 - val binary crossentropy: 0.6616 - val accuracy: 0.5710
Epoch 40/10000
.20/20 - 0s - loss: 0.6659 - AUC: 0.6798 - binary_crossentropy: 0.6583 - accuracy: 0.6102 - val_loss: 0.6715 - val_AUC: 0.6627 - val_binary_crossentropy: 0.6640 - val_accuracy: 0.5600
Epoch 41/10000
.20/20 - 0s - loss: 0.6695 - AUC: 0.6693 - binary_crossentropy: 0.6619 - accuracy: 0.6005 - val_loss: 0.6687 - val_AUC: 0.6677 - val_binary_crossentropy: 0.6611 - val_accuracy: 0.5960
Epoch 42/10000
.20/20 - 0s - loss: 0.6658 - AUC: 0.6778 - binary_crossentropy: 0.6582 - accuracy: 0.6088 - val_loss: 0.6684 - val_AUC: 0.6689 - val_binary_crossentropy: 0.6608 - val_accuracy: 0.6040
Epoch 43/10000
.20/20 - 0s - loss: 0.6655 - AUC: 0.6820 - binary crossentropy: 0.6579 - accuracy: 0.6133 - val loss: 0.6687 - val AUC: 0.6755 - val binary crossentropy: 0.6611 - val accuracy: 0.6130
Epoch 44/10000
.20/20 - 0s - loss: 0.6647 - AUC: 0.6823 - binary_crossentropy: 0.6571 - accuracy: 0.6154 - val_loss: 0.6703 - val_AUC: 0.6677 - val_binary_crossentropy: 0.6627 - val_accuracy: 0.5640
Epoch 45/10000
.20/20 - 0s - loss: 0.6683 - AUC: 0.6748 - binary_crossentropy: 0.6607 - accuracy: 0.6062 - val_loss: 0.6668 - val_AUC: 0.6685 - val_binary_crossentropy: 0.6592 - val_accuracy: 0.5850
Epoch 46/10000
.20/20 - 0s - loss: 0.6641 - AUC: 0.6851 - binary crossentropy: 0.6565 - accuracy: 0.6160 - val loss: 0.6709 - val AUC: 0.6611 - val binary crossentropy: 0.6634 - val accuracy: 0.5570
Epoch 47/10000
.20/20 - 0s - loss: 0.6652 - AUC: 0.6834 - binary_crossentropy: 0.6576 - accuracy: 0.6083 - val_loss: 0.6642 - val_AUC: 0.6828 - val_binary_crossentropy: 0.6566 - val_accuracy: 0.6030
Epoch 48/10000
.20/20 - 0s - loss: 0.6643 - AUC: 0.6824 - binary_crossentropy: 0.6567 - accuracy: 0.6135 - val_loss: 0.6669 - val_AUC: 0.6837 - val_binary_crossentropy: 0.6593 - val_accuracy: 0.6250
Epoch 49/10000
.20/20 - 0s - loss: 0.6629 - AUC: 0.6880 - binary_crossentropy: 0.6553 - accuracy: 0.6212 - val_loss: 0.6694 - val_AUC: 0.6833 - val_binary_crossentropy: 0.6618 - val_accuracy: 0.6280
.20/20 - 0s - loss: 0.6671 - AUC: 0.6707 - binary crossentropy: 0.6595 - accuracy: 0.6022 - val loss: 0.6670 - val AUC: 0.6635 - val binary crossentropy: 0.6594 - val accuracy: 0.5760
Epoch 51/10000
.20/20 - 0s - loss: 0.6632 - AUC: 0.6886 - binary_crossentropy: 0.6556 - accuracy: 0.6222 - val_loss: 0.6680 - val_AUC: 0.6651 - val_binary_crossentropy: 0.6604 - val_accuracy: 0.5710
.20/20 - 0s - loss: 0.6633 - AUC: 0.6834 - binary_crossentropy: 0.6557 - accuracy: 0.6178 - val_loss: 0.6617 - val_AUC: 0.6904 - val_binary_crossentropy: 0.6541 - val_accuracy: 0.6060
Epoch 53/10000
.20/20 - 0s - loss: 0.6635 - AUC: 0.6873 - binary_crossentropy: 0.6559 - accuracy: 0.6146 - val_loss: 0.6639 - val_AUC: 0.6857 - val_binary_crossentropy: 0.6563 - val_accuracy: 0.5980
Epoch 54/10000
.20/20 - 0s - loss: 0.6613 - AUC: 0.6897 - binary crossentropy: 0.6537 - accuracy: 0.6216 - val loss: 0.6662 - val AUC: 0.6790 - val binary crossentropy: 0.6586 - val accuracy: 0.5960
Epoch 55/10000
.20/20 - 0s - loss: 0.6618 - AUC: 0.6899 - binary_crossentropy: 0.6542 - accuracy: 0.6244 - val_loss: 0.6647 - val_AUC: 0.6841 - val_binary_crossentropy: 0.6571 - val_accuracy: 0.6200
Epoch 56/10000
.20/20 - 0s - loss: 0.6632 - AUC: 0.6903 - binary_crossentropy: 0.6555 - accuracy: 0.6234 - val_loss: 0.6673 - val_AUC: 0.6757 - val_binary_crossentropy: 0.6597 - val_accuracy: 0.5720
Epoch 57/10000
.20/20 - 0s - loss: 0.6613 - AUC: 0.6948 - binary crossentropy: 0.6537 - accuracy: 0.6284 - val loss: 0.6631 - val AUC: 0.6788 - val binary crossentropy: 0.6555 - val accuracy: 0.5880
.20/20 - 0s - loss: 0.6585 - AUC: 0.7015 - binary crossentropy: 0.6508 - accuracy: 0.6348 - val loss: 0.6667 - val AUC: 0.6812 - val binary crossentropy: 0.6590 - val accuracy: 0.5810
Epoch 59/10000
.20/20 - 0s - loss: 0.6602 - AUC: 0.6943 - binary_crossentropy: 0.6526 - accuracy: 0.6260 - val_loss: 0.6622 - val_AUC: 0.6891 - val_binary_crossentropy: 0.6545 - val_accuracy: 0.6100
Epoch 60/10000
.20/20 - 0s - loss: 0.6636 - AUC: 0.6824 - binary crossentropy: 0.6560 - accuracy: 0.6228 - val loss: 0.6743 - val AUC: 0.6526 - val binary crossentropy: 0.6667 - val accuracy: 0.5340
```

```
Epoch 61/10000
.20/20 - 0s - loss: 0.6658 - AUC: 0.6721 - binary_crossentropy: 0.6582 - accuracy: 0.6052 - val_loss: 0.6626 - val_AUC: 0.6767 - val_binary_crossentropy: 0.6550 - val_accuracy: 0.6010
Epoch 62/10000
.20/20 - 0s - loss: 0.6574 - AUC: 0.7022 - binary_crossentropy: 0.6498 - accuracy: 0.6360 - val_loss: 0.6627 - val_AUC: 0.6841 - val_binary_crossentropy: 0.6551 - val_accuracy: 0.5990
```

1 size_histories['paper'].history['AUC'][0:10]

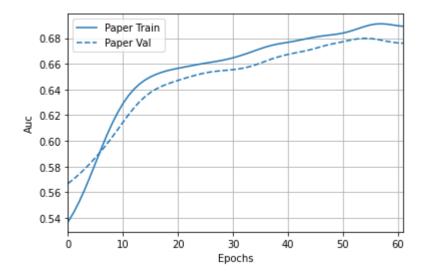
- [0.5014192461967468, 0.5259501934051514, 0.5493761897087097, 0.567119836807251,
- 0.5775632858276367, 0.5930601954460144, 0.6003478765487671, 0.6114186644554138, 0.6216607093811035,
- 0.6321367621421814]

 1 plotter = tfdocs.plots.HistoryPlotter(metric = 'binary_crossentropy', smooth
- 1 plotter = tfdocs.plots.HistoryPlotter(metric = 'binary_crossentropy', smoothing_std=10)
 2 plotter.plot(size_histories)
 3 # plt.ylim([0.5, 0.7])
 - 0.695 0.690 0.685 0.680 0.675 0.675 0.660 0.665 0.660

20

1 plotter = tfdocs.plots.HistoryPlotter(metric = 'AUC', smoothing_std=10)
2 plotter.plot(size_histories)
3 # plt.ylim([0.5, 0.7])

30 Epochs



▼ Plot the training and validation losses

The solid lines show the training loss, and the dashed lines show the validation loss (remember: a lower validation loss indicates a better model).

While building a larger model gives it more power, if this power is not constrained somehow it can easily overfit to the training set.

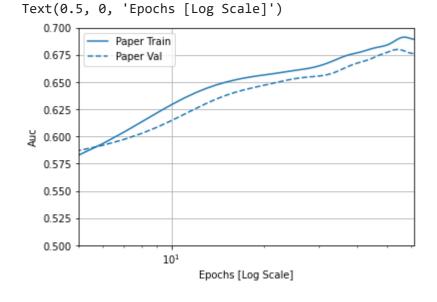
In this example, typically, only the "Tiny" model manages to avoid overfitting altogether, and each of the larger models overfit the data more quickly. This becomes so severe for the "large" model that you need to switch the plot to a log-scale to really see what's happening.

This is apparent if you plot and compare the validation metrics to the training metrics.

- It's normal for there to be a small difference.
- If both metrics are moving in the same direction, everything is fine.
- If the validation metric begins to stagnate while the training metric continues to improve, you are probably close to overfitting.
- If the validation metric is going in the wrong direction, the model is clearly overfitting.

```
1 plotter.plot(size_histories)
2 a = plt.xscale('log')
3 plt.xlim([5, max(plt.xlim())])
4 plt.ylim([0.5, 0.7])
5 plt xlabel("Epochs [Log Scale]")
```

5 plt.xlabel("Epochs [Log Scale]")



Note: All the above training runs used the callbacks. EarlyStopping to end the training once it was clear the model was not making progress.

▼ View in TensorBoard

These models all wrote TensorBoard logs during training.

To open an embedded TensorBoard viewer inside a notebook, copy the following into a code-cell:

%tensorboard --logdir {logdir}/sizes

You can view the <u>results of a previous run</u> of this notebook on <u>TensorBoard.dev</u>.

TensorBoard.dev is a managed experience for hosting, tracking, and sharing ML experiments with everyone.

It's also included in an <iframe> for convenience:

1 display.IFrame(
2 src="https://tensorboard.dev/experiment/vW7jmmF9TmKmy3rbheMQpw/#scalars&_smoothingWeight=0.97",
3 width="100%", height="800px")

•

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TensorBoard.dev

SCALARS GRAPHS HISTOGRAMS DISTRIBUTIONS HPARAMS SEND FEEDBACK

If you want to share TensorBoard results you can upload the logs to <u>TensorBoard.dev</u> by copying the following into a code-cell.

Note: This step requires a Google account.

small/validation

!tensorboard dev upload --logdir {logdir}/sizes

Caution: This command does not terminate. It's designed to continuously upload the results of long-running experiments. Once your data is uploaded you need to stop it using the "interrupt execution" option in your notebook tool.

