Business 4720 - Class 15

Neural Networks using Python

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This Class

What You Will Learn:

- Deep Learning Concepts
  - Neural Network
  - Activation Functions
  - Gradients
  - Backpropagation
  - Regularization with Dropouts
- Deep Learning in Python using Tensoflow
  - Tensors
  - Models
  - Training

Based On

Gareth James, Daniel Witten, Trevor Hastie and Robert Tibshirani: *An Introduction to Statistical Learning with Applications in R*. 2nd edition, corrected printing, June 2023. (ISLR2)

`https://www.statlearning.com`

Chapter 10

Kevin P. Murphy: *Probabilistic Machine Learning – An Introduction*. MIT Press 2022.

`https://probml.github.io/pml-book/book1.html`

Chapter 13, 14, 15

Tensorflow Guides

`https://www.tensorflow.org/guide`

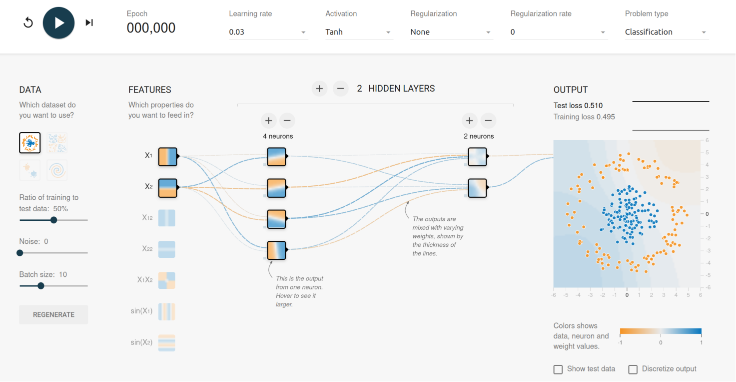
Resources

Implementations are available on the following GitHub repo:
`https://github.com/jevermann/busi4720-ml`

The project can be cloned from this URL:
`https://github.com/jevermann/busi4720-ml.git`

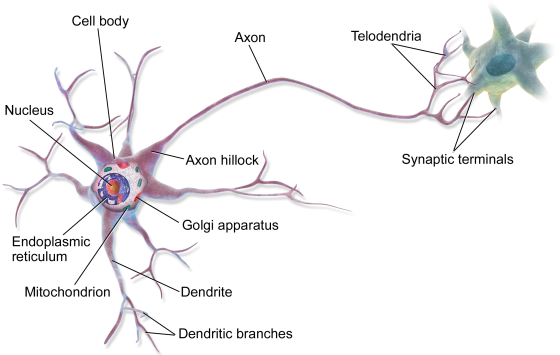
Resources

Tensorflow Playground: `https://playground.tensorflow.org`



Biological Neuron

- Brain cell
- Connected to other brain cells
- Receives, modulates and emits electro-chemical stimulus (”activation”)



https://commons.wikimedia.org/wiki/File:Blausen_0657_MultipolarNeuron.png

Artificial Neuron

$$y = \psi(b + \sum_i w_i x_i)$$

- Multiple **input** connections x_i
- Weighted using **weights** w_i
- Add a **bias** term b
- Apply *nonlinear* **activation function** ψ

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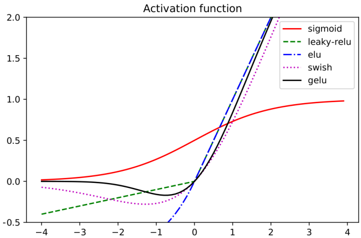
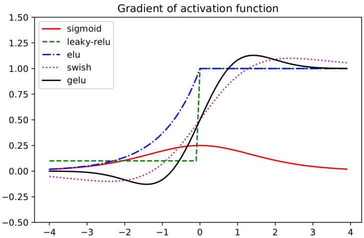
Popular Activation Functions

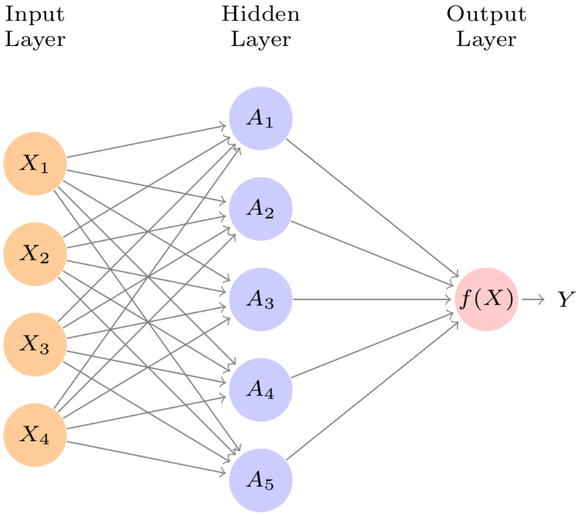
Sigmoid	$\sigma(z) = \frac{e^z}{1+e^z}$
Hyperbolic tangent	$\tanh(z) = \frac{sinh(z)}{cosh(z)} = \frac{e^z - e^{-z}}{e^z + e^{-z}} = 2\sigma(2z) - 1$
Softplus	$\sigma_+(z) = \log(1 + e^a)$
Rectified linear unit	$\text{ReLU}(z) = \max(a, 0)$
Leaky ReLU	$\text{LReLU}(z) = \max(z, 0) + \alpha \min(z, 0)$
Exponential linear unit	$\text{ELU}(z) = \max(z, 0) + \min(\alpha(e^z - 1), 0)$
Swish, Sigmoid linear unit	$\text{SiLU}(z) = z\sigma(z)$
Gaussian error linear unit	$\text{GeLU}(z) = z\Phi(z)$





Source: Murphy, Fig. 13.14

Fully Connected Hidden Layer



Source: ISLR2 Figure 10.1

Counting Parameters

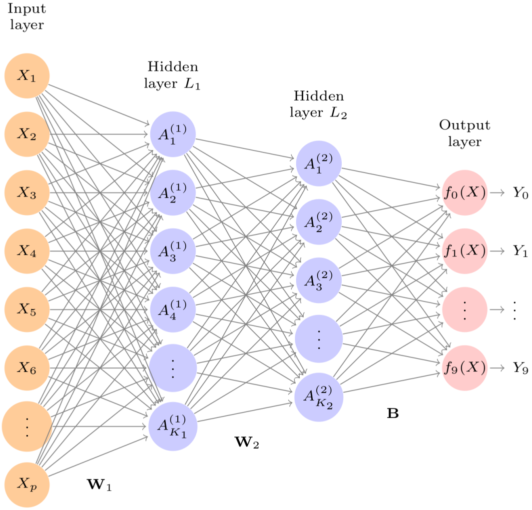
In a fully-connected network, for a hidden or output layer of size n, that is, with n cells/neurons and k inputs, that is k cells on the previous layer:

- Each of the n cells has as many weights as inputs k
- Each of the n cells has 1 bias

Example: Input size 4, hidden layer size 5, output layer size 1:

- Hidden layer parameters: $4 \times 5 + 5 = 25$
- Ouput layer parameters: $5 \times 1 + 1 = 6$
- Total number of parameters: $25 + 6 = 31$

Fully Connected Multilayer Network



Source: ISLR2 Figure 10.4

Multiple Outputs either

- Multi-objective learning
- Multi-class classification

"**Softmax**" activation

$$\Pr(Y = m|X) = \frac{e^{Z_m}}{\sum_{l=0}^{n} e^{Z_l}}$$

Hands-On Exercise

Consider the following network architecture for classification into 5 classes.

- Input layer with 10 inputs
- Fully-connected (dense) hidden layer with 20 units
- Fully-connected (dense) hidden layer with 10 units
- Fully-connected (dense) hidden layer with 5 units
- Fully-connected (dense) output layer

Calculate the total number of learnable parameters for this network.

Estimating Parameters

Typical Loss Functions

- **Regression**: MSE, MAE, Huber
- **Classification**: Cross-Entropy or KL-Divergence after softmax on multiple output nodes

Parameters

- Parameter vector $\theta = (w, b)$ with weights w and biases b.

Optimization

- (Stochastic) gradient descent (SGD)

Regularization

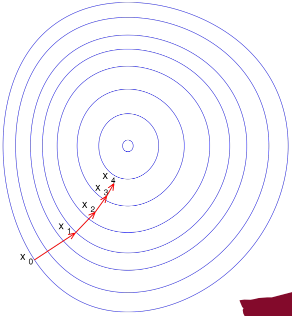
- ”Dropout”
- L1 and/or L2 penalization (as in lasso, ridge)
- Early stopping

Gradient Descent

1. Begin with initial parameter values
2. Repeat until convergence
   2.1 Find direction of descent (decrease in loss function value, given by the gradient vector ∇L of partial derivatives)
   2.2 Move a step in that direction (adjust parameters, step size determined by **learning rate**)

Consider the loss L at a certain input X as a function of parameter values θ. Then, at each step t, update parameters θ using learning rate γ:

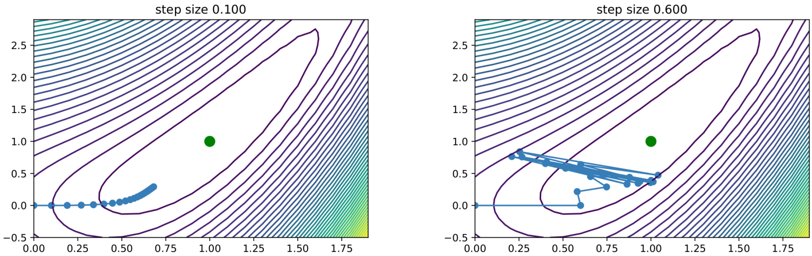
$$\theta_{t+1} = \theta_t - \gamma \nabla L(\theta)|_{\theta_t, X}$$



https://commons.wikimedia.org/wiki/File:Gradient_descent.svg

Optimization Problems

- Slow convergence
- No convergence (oscillations)
- Premature convergence (local optimimum)



Murphy, Figure 8.11

Optimization Options

Learning Rate

- Fixed step size
- Adaptive learning rate λ_t
- Momentum methods
- Optimal learning rate (”line search”)

Training Neural Networks – Epochs and Minibatches

- Using the full training set for every update step is expensive (or impossible)
- Approximate true gradient by using a small sample of the training set for each step, the **minibatch**
  - Average gradients over minibatch
  - Minibatch should be independent and random
  - Minibatch size should not be ”too small”
- Multiple passes over the training set until convergence (a local or global optimimum is found), the **epochs**
  - Avoid repetition by shuffling the training set before each epoch
  - Early stopping for regularization

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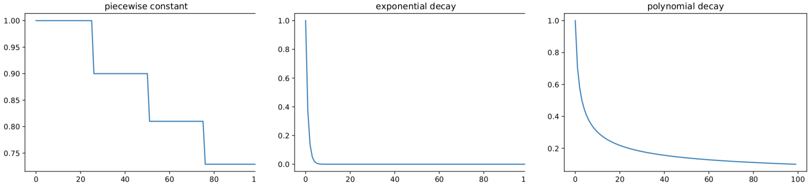
Optimization Options – Stochastic Gradient Descent

- Random inputs X to gradients by random draws from training set

$$\theta_{t+1} = \theta_t - \lambda_t \nabla L(\theta)|_{\theta_t, X}$$

- Requires adaptive learning rate
- Typical learning rate schedules: Piecewise constant, exponential decay, polynomial decay



Source: Murphy Figure 8.18

Optimization Options – AdaGrad

Adaptive Gradient

- Originally developed for sparse gradient vectors
- Adapt by previous squared gradients
- Overall learning rate λ_t is adapted
- Typically: $\lambda_t = \lambda_0$

$$\theta_{t+1} = \theta_t - \lambda_t \frac{1}{\sqrt{s_t + \epsilon}} \nabla L(\theta)|_{\theta_t, X}$$

$$s_t = \sum_{\tau=1}^{t} \left(\nabla L(\theta)|_{\theta_\tau, X} \right)^2 \quad \text{Sum of squared gradients}$$

Optimization Options – RMSProp

- Exponentially weighted moving average of the past (instead of the sum as in AdaGrad)
- Prevents too early learning rate reduction

$$s_{t+1} = \beta s_t + (1 - \beta) \left(\nabla L(\theta)|_{\theta_t, X} \right)^2$$

Optimization Options – AdaDelta

- Maintains exponentially weighted average of previous updates δ

$$
\begin{aligned}
\theta_{t+1} &= \theta_t + \Delta\theta_t \\
\Delta\theta_t &= -\lambda_t \frac{\sqrt{\delta_{t-1} + \epsilon}}{\sqrt{s_t + \epsilon}} \nabla L(\theta)|_{\theta_t, x} \\
\delta_t &= \beta\delta_{t-1} + (1 - \beta)(\Delta\theta_t)^2
\end{aligned}
$$

Optimization Options – Momentum Methods

- *Intuition*: Keep going in the direction that was previously good, avoid ”sharp turns”
- Standard momentum:

$$m_{t+1} = \beta m_t - \nabla L(\theta)|_{\theta_t, X} \qquad \text{Momentum}$$
$$\theta_{t+1} = \theta_t - \lambda m_{t+1} \qquad \text{Parameter update}$$

Typical β is ≈ 0.9

- Nesterov Momentum: Looks ahead and evaluates gradient at approximate next parameter values

$$m_{t+1} = \beta m_t - \lambda_t \nabla L(\theta)|_{\theta_t + \beta m_t, X} \qquad \text{Nesterov Momentum}$$
$$\theta_{t+1} = \theta_t + m_{t+1} \qquad \text{Parameter update}$$

Optimization Options – AdaM

Adaptive Moment Estimation

- Combine adaptive learning rate with momentum

$$
\begin{aligned}
m_t &= \beta_1 m_{t-1} + (1-\beta_1)\nabla L(\theta)|_{\theta_t,X} \\
s_t &= \beta_2 s_{t-1} + (1-\beta_2)\left(\nabla L(\theta)|_{\theta_t,x}\right)^2 \\
\theta_{t+1} &= \theta_t - \lambda_t \frac{1}{\sqrt{s_t}+\epsilon} m_t
\end{aligned}
$$

Training Neural Networks – Vanishing Gradients

Problem

- Sigmoid and tanh functions are bounded for large positive or negative pre-activation values (”saturating activation functions”)
- Long chains of neurons (e.g. in stacked fully-connected layers) can diminish the ”error signal”, i.e. the gradient

Possible Solutions

- Use non-saturating activation functions, e.g. ReLU, leaky ReLU, ELU, etc.
- Use additive rather multiplicative architectures, e.g. ”ResNet” (residual networks)
- Standardize activations at every layer
- Carefully choose initial parameter values

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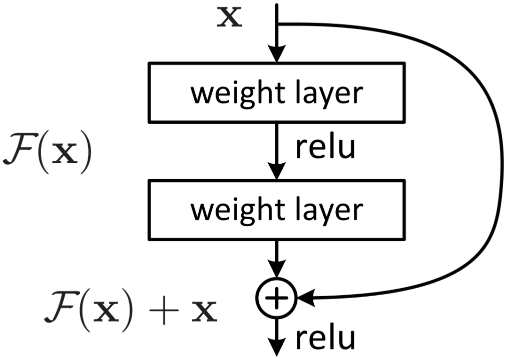
- Allows gradients to bypass a layer that suffers from lack of learning (vanishing gradient, saturated activation)



Source: Murphy, Figure 13.15

Training Neural Networks – Exploding Gradients

Problem

- Long chains of neurons can vastly increase the error

Possible Solution

- Gradient clipping

$$g' = min(1, \frac{1}{||c||_2})g$$

Training Neural Networks – Parameter Initialization Heuristics

- Random values from normal distribution: $\theta \sim N(0, \sigma^2)$
- "Xavier Initialization"/"Glorot Initialization"

$$\sigma^2 = \frac{2}{n_{\text{in}} + n_{\text{out}}}$$

where n_{in} is the number of incoming connections and n_{out} is the number of outgoing connections from each neuron

- "LeCun Initialization"

$$\sigma^2 = \frac{1}{n_{\text{in}}}$$

- "He Initialization"

$$\sigma^2 = \frac{2}{n_{\text{in}}}$$

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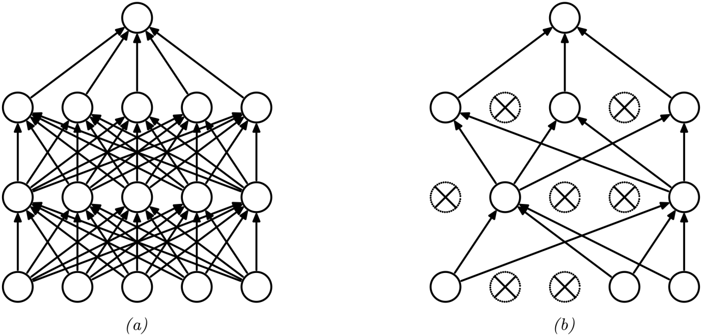
Regularization – Dropout

- Randomly (per observation) remove a fraction of units in a layer, or equivalently,
- Randomly set the output of a fraction of units to 0
- Typically only done at train time, not test time



Source: Murphy, Figure 1.318

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TensorFlow

- Originally developed by Google, Version 1.0 in 2017
- Automatic differentiation/gradients
- Distributed computing
- Parallel computing on multiple GPU
- Wide range of loss functions
- Wide range of optimizers
- Wide range of neural network types and activation functions

Keras

- Originally developed as a user-friendly, high-level abstraction layer for different ML frameworks, including Tensorflow, Theano, PyTorch
- Wide range of standard neural network layers
- Simplified training loops

Regression using Keras

Import required packages:

```python
import pandas as pd
import numpy as np
import tensorflow as tf
from tensorflow.keras import layers
```

Read a CSV file:

```python
# Use the Boston housing data set
boston_data = \
    pd.read_csv("https://evermann.ca/busi4720/boston.csv")
```

Separate features and target:

```python
boston_features = boston_data.copy()
boston_labels = boston_features.pop('medv')
```

Define the NN model with one hidden fully-connected layer (64 neurons) and one fully-connected output layer (1 neuron) in sequence. No activation function is given, so this is a linear regression model:

```python
boston_model = tf.keras.Sequential([
  layers.Dense(64, activation=None),
  layers.Dense(1, activation=None)
])
```

Set the loss function and the optimizer:

```python
boston_model.compile(
    loss = tf.keras.losses.MeanSquaredError(),
    optimizer = tf.keras.optimizers.Adam())
```

Fit/train the model for 25 epochs:

```python
boston_model.fit(boston_features,
                 boston_labels, epochs=25)
boston_model.summary()
```

Regression in Keras [cont'd]

The `Normalization` layer normalizes numeric features:

```python
norm_layer = layers.Normalization()
```

The `adapt()` function computes means and variances of the data so the layer can normalize the data when the model is fit. Requires numpy array.

```python
norm_layer.adapt(boston_features.to_numpy())
```

Add the normalization layer to the model. A ReLU activation is used that makes this a non-linear regression model:

```python
norm_boston_model = tf.keras.Sequential([
  norm_layer,
  layers.Dense(64, activation='relu'),
  layers.Dense(1, activation=None)
])
```

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Regression in Keras [cont'd]

Set loss and optimizer and ask Keras to keep track of the MSE and MAE metrics.

Python
```python
norm_boston_model.compile(
    loss = tf.keras.losses.MeanSquaredError(),
    optimizer = tf.keras.optimizers.Adam(),
    metrics = ['mse', 'mae'])
```

The `fit` function returns a history of the metrics we asked for:

Python
```python
train_hist = \
    norm_boston_model.fit(
        boston_features,
        boston_labels,
        batch_size=20,
        epochs=50,
        validation_split=0.33)
```

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Plot the training history using Plotly Express

Python
```
import plotly.express as px

hist = pd.DataFrame({
    'training': train_hist.history['mse'],
    'validation': train_hist.history['val_mse']})
hist['epoch'] = np.arange(hist.shape[0])
hist = pd.melt(hist,
               id_vars='epoch',
               value_vars=['training', 'validation'])

fig = px.line(hist, x='epoch', y='value',
                    color='variable')
fig.show()
```

Hands-On Exercises

- Modify the above code to include different activation functions, e.g. `"tanh"`, `"sigmoid"`, or `"elu"`. Comment on the learning progress and loss function values.
- Modify the above code to change the number of neurons in the `"Dense"` layer. Comment on the learning progress and loss function values.
- Modify the architecture to add one or more `"Dense"` layers with different numbers of units. Comment on the learning progress and loss function values.

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Classification in Keras

The `Wage` dataset from the ISLR2 library for R has been adapted to include a column `wagequart`, the quartile of the wage. Many features are categorical.

Python

```
# Read data and separate features from target labels
wage_data = \
    pd.read_csv("https://evermann.ca/wage.csv")

wage_features = wage_data.copy()
wage_labels = wage_features.pop('wagequart') - 1
```

Treat each categorical string feature and convert to **one-hot encoding**.

One-hot encoding is similar to binary dummy variables (contrasts) in linear models, but have no default level; a feature with n different categories requires n binary variables (not $n - 1$ as in linear model contrasts).

Keep track of the inputs and the pre-processed inputs:

Python
```
inputs = {}
preproc_inputs = []
```

Classification in Keras [cont'd]

Python
```
for cat_feature in ['maritl', 'race', 'education', \
                    'jobclass', 'health', 'health_ins']:
    # An Input variable is a placeholder that
    # accepts data input when training or predicting
    input = tf.keras.Input(shape=(1,),
                           name=cat_feature,
                           dtype=tf.string)
    # This StringLookup layer accepts a string and
    # outputs its category as a one-hot vector
    lookup = layers.StringLookup(
        name=cat_feature+"_lookup",
        output_mode="one_hot")
    # Adapt it to the different strings in the data
    lookup.adapt(wage_features[cat_feature])
    # And tie the input to this layer
    onehot = lookup(input)

    inputs[cat_feature] = input
    preproc_inputs.append(onehot)
```

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Classification in Keras [cont'd]

Define and input and a `Normalizaton` layer for the numerical variable `age`:

```python
age_input = tf.keras.Input(shape=(1,),
                           name="age",
                           dtype="float32")
norm_layer = layers.Normalization(name="age_norm")
norm_layer.adapt(wage_features["age"])
age_norm = norm_layer(age_input)

inputs["age"] = age_input
preproc_inputs.append(age_norm)
```

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Classification in Keras [cont'd]

Define and input and a one-hot encoding `IntegerLookup` layer for the numeric variable `year`:

```python
year_input = tf.keras.Input(shape=(1,),
                            name="year",
                            dtype="int32")
lookup = layers.IntegerLookup(name="year_lookup",
                              output_mode="one_hot")
lookup.adapt(wage_features["year"])
year_onehot = lookup(year_input)

inputs["year"] = year_input
preproc_inputs.append(year_onehot)
```

Concatenate the pre-processing outputs to one long vector with a `Concatenate` layer. Call this layer with the list of prec-processed inputs:

Python
```
preprocessed_inputs = \
    layers.Concatenate(name="concat")(preproc_inputs)
```

Build a pre-processing model whose inputs is the dict of `Input` variables, and whose output are the results of calling the layers:

Python
```
preproc_model = tf.keras.Model(inputs,
                               preprocessed_inputs,
                               name="preproc")
preproc_model.summary()
```

Classification in Keras [cont'd]

Build the classification model as a `Sequential` model:

```python
class_model = tf.keras.Sequential(name="classification")
class_model.add(layers.Dense(64, activation="relu"))
class_model.add(layers.Dropout(0.25))
class_model.add(layers.Dense(32, activation="relu"))
class_model.add(layers.Dropout(0.25))
class_model.add(layers.Dense(4, activation="softmax"))

# Alternatively:
# class_model.add(layers.Dense(4, activation=None))
# class_model.add(layers.Softmax())
```

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Classification in Keras [cont'd]

The output of the pre-processing model is the input to the classification model:

```python
class_results = class_model(preproc_model(inputs))
class_model.summary()
```

The final model takes the inputs, and has the classification model results as outputs:

```python
wage_model = tf.keras.Model(inputs, class_results,
                            name="wage_model")
wage_model.summary()
```

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Classification in Keras [cont'd]

Compile the model with loss function, optimizer and request training metrics:

```python
wage_model.compile(
    loss=tf.keras.losses.SparseCategoricalCrossentropy(
       from_logits=False),
    optimizer=tf.keras.optimizers.Adam(
        learning_rate=0.001,
        beta_1 = 0.9,
        beta_2 = 0.999,
        epsilon = 1e-07),
    metrics=[
        tf.keras.metrics.SparseCategoricalAccuracy(),
        tf.keras.metrics.KLDivergence()])
```

Note: Specifying `from_logits=True` for the loss can save the softmax activation or layer at the bottom of the sequential classification model.

Create the input data as a dict of numpy arrays to match the `Input` variables:

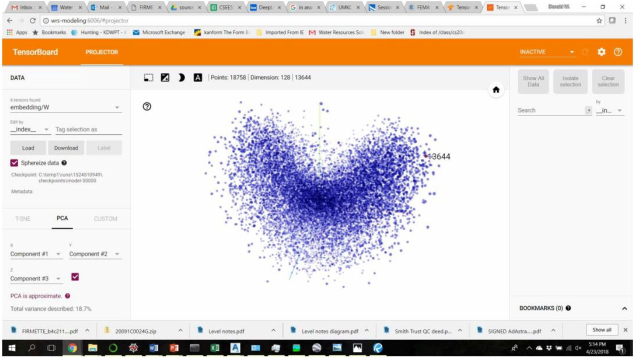
```python
import numpy as np
wage_feature_dict = \
    {name: np.array(value) for \
        name, value in wage_features.items()}
```

Write log information to a directory for loading into **Tensorboard**:

```python
import datetime
log_dir = "./tensorboard_logs/" + \
    datetime.datetime.now().strftime("%Y%m%d-%H%M%S")
tensorboard_callback = \
    tf.keras.callbacks.TensorBoard(log_dir=log_dir,
        histogram_freq=0)
```

TensorBoard

TensorBoard is a tool to visualize neural network models and their trainging and validation data/performance.



https://commons.wikimedia.org/wiki/File:Tensorboard_1.jpg

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Classification in Keras [cont'd]

Train the model for 25 epochs:

```python
wage_hist = wage_model.fit(
    x = wage_feature_dict,
    y = wage_labels,
    validation_split=0.333,
    batch_size=20,
    epochs = 25,
    callbacks=[tensorboard_callback])
```

Plot the training history using Plotly Express

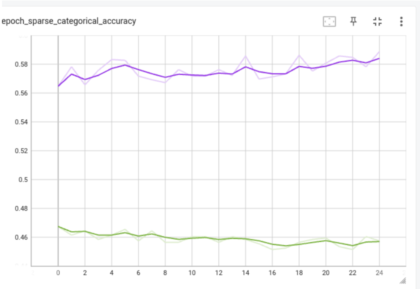
Python
```
import plotly.express as px

hist = pd.DataFrame({
    'training': \
wage_hist.history['sparse_categorical_accuracy'],
    'validation': \
wage_hist.history['val_sparse_categorical_accuracy']})
hist['epoch'] = np.arange(hist.shape[0])
hist = pd.melt(hist,
               id_vars='epoch',
               value_vars=['training', 'validation'])

fig = px.line(hist, x='epoch', y='value',
                    color='variable')
fig.show()
```

Classification in Keras [cont'd]

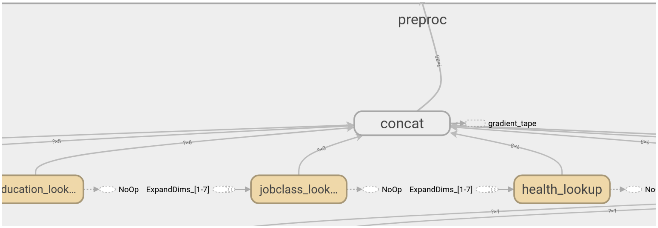
Call TensorBoard from the terminal, providing the log directory

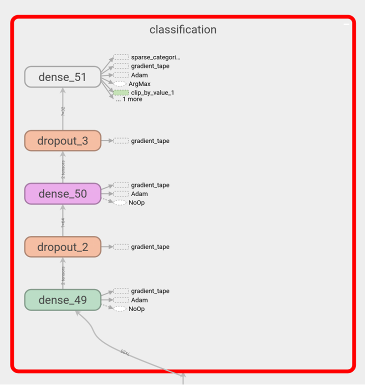
Bash
```bash
tensorboard --logdir tensorboard_logs
```

Then go to `http://localhost:6006` in your web browser.



TensorBoard





Early Stopping

Another useful callback function:

Python
```
earlystop_callback = tf.keras.callbacks.EarlyStopping(
    monitor = 'val_loss',
    patience = 3,
    mode = 'min',
    # or 'max' or 'auto' depending on monitor metric
    restore_best_weights = True)
```

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Hands-On Exercises

- Examine the model summaries for the pre-processing, the classification, and the complete wage model. Explain the number of trainable and total parameters, and also explain the output shapes of each layer.
- Make the ”wage” prediction a binary classification problem:

1. Modify the `wage_labels` and combine classes 0, 1 and classes 2, 3 (class numbers should be 0 or 1)
2. Modify the classification network to have a single output node
3. Use the `BinaryCrossentropy` loss
4. Return the following metrics as part of the training history:
   - Precision
   - Recall
   - AUC
5. Plot the metrics after training