Functional model: the basics

The `Sequential` model

- organizes layers as an ordered list
- restricts the input to layer $(l+1)$ to be the output of layer l.

The computation of a Sequential model is easy to describe and picture

- a graph
- each node represents the computation of a layer
- the nodes are connected sequentially in a straight line
- single input, single output
    - mostly true
    - can have inputs/outputs that are arrays, each element representing a different input/output value

The Functional model

- imposes **no** ordering on layers
- imposes **no** restriction on connect outputs of one layer to the input of another

The computation of a Functional model can be pictured as a general graph

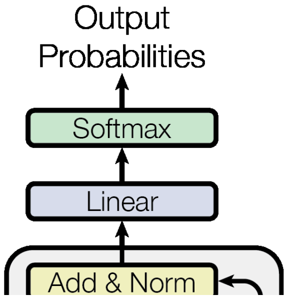
- each node represents a computation
- edges can flow from any node to any other
    - non-cyclic
- multiple inputs, multiple outputs possible

To illustrate the `Functional` model let's take a first look at model implementing a single `Transformer` block

- we will revisit this code later to illustrate other concepts

Here is the picture of a Transformer block

Transformer (Encoder/Decoder)


Output
Probabilities
Softmax
Linear
Add & Norm

We can identify some connections that *don't* flow sequentially between adjacent nodes

- the *skip connection* that bypasses
    - the Multi-Head Attention node in the Encoder and the top Multi-Head Attention node in the Decoder
    - the Masked Multi-Head Attention node in the Decoder
- the connection from the output of the Encoder (top left) to the input of the Decoder Multi-Head Attention node

The Functional Model architecture, in code

[reference (https://www.tensorflow.org/guide/keras/functional)](https://www.tensorflow.org/guide/keras/functional)

In the Sequential model, the output of the node representing layer l is *always* fed to the input of the node representing layer $(l+1)$

- So can describe the computation graph as a sequence of nodes (each node a `Layer` type)

In the Functional model a node represents a function that takes one or more inputs and produces an output

- the node does not need to be a `Layer`
    - any TensorFlow `op`
- we connect the output of node $\mathbb{N}_\mathrm{a}$ to the input of node $\mathbb{N}_\mathrm{b}$
    - by assigning the output of $\mathbb{N}_\mathrm{a}$ to a variable (typically denoted as `x`)
    - calling the computation of $\mathbb{N}_\mathrm{b}$ with the variable as actual parameter

Here is an example (source (https://www.tensorflow.org/api_docs/python/tf/keras/Model))

```
import tensorflow as tf

inputs = tf.keras.Input(shape=(3,))
x = tf.keras.layers.Dense(4, activation=tf.nn.relu)(inputs)
outputs = tf.keras.layers.Dense(5, activation=tf.nn.softmax)(x)
model = tf.keras.Model(inputs=inputs, outputs=outputs)
```

- There is an `Input` layer (a function with no argument) whose output is assigned to variable `inputs`
- There is a `Dense` layer (a function with a single argument and single output)
    - that is called with parameter `inputs`
    - assigns its result to variable `x`

In general, these variables could be used as arguments (i.e., node inputs) anywhere in the computation

- not necessarily the next function appearing sequentially

The collection (not necessarily a sequence) of function calls defines a *Directed Acyclic Graph*

- one or more *root* nodes representing graph inputs
- one of more *leaf* nodes representing graph outputs

The graph encodes a complex function mapping inputs to outputs, composed of simpler functions.

The graph can be used to implement

- a new `Layer`
- a complete `Model`

To turn this collection into a `Model`

- we specify the input nodes
- we specify the output nodes

For example, for the above graph:

```
model = tf.keras.Model(inputs=inputs, outputs=outputs)
```

When `model` is *called*

- the actual parameters are bound to the nodes identified as inputs
    - i.e., `inputs`
- the result of the call are the values associated with the nodes identified as
    - i.e., `outputs`\`

Since a graph can have multiple inputs and outputs

- the `input` and `output` parameters of the `Model` statement can be *lists*

[`Model` reference (https://www.tensorflow.org/api_docs/python/tf/keras/Model)](https://www.tensorflow.org/api_docs/python/tf/keras/Model)

Sub-classing models/layers

One can create a new `Model` / `Layer` by sub-classing from the base types `tf.keras.Model` / `tf.keras.layers.Layer`

- can override existing methods of a `Model`
    - e.g., a custom training step (invoked by `fit`)
- can build new `Layer` types

Here is an example (taken from [the reference (https://www.tensorflow.org/guide/keras/functional#functional_api_strengths)](https://www.tensorflow.org/guide/keras/functional#functional_api_strengths))

In [12]:

```
class MLP(keras.Model):

  def __init__(self, **kwargs):
    super(MLP, self).__init__(**kwargs)
    self.dense_1 = layers.Dense(64, activation='relu')
    self.dense_2 = layers.Dense(10)

  def call(self, inputs):
    x = self.dense_1(inputs)
    return self.dense_2(x)

# Instantiate the model.
mlp = MLP()
# Necessary to create the model's state.
# The model doesn't have a state until it's called at least once.
_ = mlp(tf.zeros((1, 32)))
```

Key points:

- Notice that the components of the `Model`
    - are instantiated in the **constructor** (`__init__`)
    - invoked in the `call`
        - the `call` method is invoked when you apply actual parameters to the `Model`

```
_ = mlp(tf.zeros((1, 32)))
```

- What would happen if you instantiated the components in the `call` ?

```
def call(self, inputs):
  x = layers.Dense(64, activation
='relu')(inputs)
  return layers.Dense(10)(x)
```

It would probably **not** be what you expected

- Instantiating the components in `__init__` results in them being defined **once**
- Instantiating the components in `call` results in them being defined separately **each time** the `Model` is called
    - weights **are not shared** between component instances
    - `call` is invoked for each step in training
        - would not learn weights of the component since they would be initialized for each batch of examples

Sub-classing Layer types is almost identical.

We will see this explicitly in our study of the code for the Transformer but here is a preview

- `init` method defines the components of the layer
- `call` method is invoked when the layer is "called"
    - uses the components defined in the `init`

Illustration of sub-classing a Layer

```
class TransformerEncoder(layers.Layer):
    def __init__(self, embed_dim, dense_dim, num_heads, **kwargs):
        super().__init__(**kwargs)
        self.embed_dim = embed_dim
        self.dense_dim = dense_dim
        self.num_heads = num_heads
        self.attention = layers.MultiHeadAttention(
            num_heads=num_heads, key_dim=embed_dim
        )
        self.dense_proj = keras.Sequential(
            [
                layers.Dense(dense_dim, activation="relu"),
                layers.Dense(embed_dim),
            ]
        )
        self.layernorm_1 = layers.LayerNormalization()
        self.layernorm_2 = layers.LayerNormalization()
        self.supports_masking = True

    def call(self, inputs, mask=None):
```

Residual/skip connection

We observe (in passing for now, more detail to come)

- two curious statements in the `call` above
    - `proj_input = self.layernorm_1(inputs + attention_output)`
    - `return self.layernorm_2(proj_input + proj_output)`

What is curious about are the two addends in the addition

- the left addend is the *input* to the previous layer
- the right addend it the *output* of the previous layer

That is

- we are adding the input and outputs of a layer together !

This is called a *Residual* (or *Skip* connection)

We will subsequently review the purpose of Residual connections.

For now

- this connection is *only possible* using the Functional architecture

Fitting a model with multiple inputs, multiple outputs

There is a technical question as to how we distinguish among the `Input` s so we can connect it to the desired variable.

In our basic introduction to Keras, the `fit` method described its training data simply

- Two `numpy` arrays: one for features, one for labels
    - an element of the first array are features of a single example
    - an element of the second array is the label of a single example (for supervised learning)

A careful examination of the [`fit` method (https://keras.io/api/models/model_training_apis/#fit-method)](https://keras.io/api/models/model_training_apis/#fit-method) describes *multiple* ways to pass train examples (and labels) to a model

- The common `x= .., y=..`
    - In its simplest form:
        - `x` and `y arenumpy`` arrays (one element per example)
- More general form
    - both the `x` and `y` can be lists
        - Functional models may define multiple *positional* (first, second, etc.) inputs and outputs
        - The `x` list: one element per input
        - The `y` list: one element per output
        - models with multiple unnamed inputs or model outputs
    - `x` can be a `dict`
        - A Functional model with multiple *named* inputs
        - the keys of the `dict` are the names of the inputs
- Tensors
    - can pass the Tensor to a *non-`Input`* layer
- `Dataset`
- Generator
    - for (feature, label) pairs when training

Specifying batches

Also: remember that Models process *batches* of examples (in fitting and predicting

- So the variables passed to `Input` layers should be *groups* of examples, not a single example
    - a single example is represented as a group of size 1

Creating batches is **done for you** when using the common `x= .., y=.., batch_size=..` calling method

- The `Dataset` **needs to create the batches** when used as the calling method
    - there is always a "batch" dimension, even if the batch size is 1
    - there is no `batch_size` argument when the inputs are `Dataset`'s
    - we will learn about the `batch` operator for transforming an un-batched `Dataset` into one with batches

Example: Multiple Loss functions from multiple outputs

In discussing multiple outputs, we skipped over an important point

- Loss is associated with an output
- When there are multiple outpus
    - there is a separate loss per output

Technical issue

- How do we specify the loss per output
- How do we combine multiple losses into a single loss, for training

Referring back to our example of multiple inputs/outputs (solving for priority and department)

- we specify a loss for each output
    - with a `dict` that maps a node name to a loss
    - the outputs have been named "priority" and "department"

```
  priority_pred = layers.Dense
(1, name="priority")(x)
  department_pred = layers.Den
se(num_departments, name="depa
rtment")(x)
```

Note how in the `fit` call

- we identify the multiple inputs by the names of their `Input` nodes
- using a `dict` as parameter

In [13]:

```
model.compile(
    optimizer=keras.optimizers.RMSprop(1e-3),
    loss={
        "priority": keras.losses.BinaryCrossentropy(from_logits=True),
        "department": keras.losses.CategoricalCrossentropy(from_logits=True),
    },
    loss_weights={"priority": 1.0, "department": 0.2},
)
```

Note the `loss_weights` parameter

- specifying the relative weight of each loss within the total loss

Here is the call to fit the model:

In [14]:

```python
# Dummy input data
title_data = np.random.randint(num_words, size=(1280, 10))
body_data = np.random.randint(num_words, size=(1280, 100))
tags_data = np.random.randint(2, size=(1280, num_tags)).astype("float32")

# Dummy target data
priority_targets = np.random.random(size=(1280, 1))
dept_targets = np.random.randint(2, size=(1280, num_departments))

model.fit(
    {"title": title_data, "body": body_data, "tags": tags_data},
    {"priority": priority_targets, "department": dept_targets},
    epochs=2,
    batch_size=32,
)
```

```
Train on 1280 samples
Epoch 1/2
WARNING:tensorflow:Entity <function Function._initialize_uninitialized_variabl
es.<locals>.initialize_variables at 0x7f70980b4290> could not be transformed a
nd will be executed as-is. Please report this to the AutoGraph team. When fili
ng the bug, set the verbosity to 10 (on Linux, `export AUTOGRAPH_VERBOSITY=10
`) and attach the full output. Cause: No module named 'tensorflow_core.estimat
or'
WARNING: Entity <function Function._initialize_uninitialized_variables.<locals
>.initialize_variables at 0x7f70980b4290> could not be transformed and will be
executed as-is. Please report this to the AutoGraph team. When filing the bug,
set the verbosity to 10 (on Linux, `export AUTOGRAPH_VERBOSITY=10`) and attach
the full output. Cause: No module named 'tensorflow_core.estimator'
1280/1280 [==============================] - 5s 4ms/sample - loss: 1.3097 - pr
iority_loss: 0.7047 - department_loss: 3.0254
Epoch 2/2
1280/1280 [==============================] - 2s 1ms/sample - loss: 1.2833 - pr
iority_loss: 0.7037 - department_loss: 2.8980
```

Out[14]: <tensorflow.python.keras.callbacks.History at 0x7f705805a950>

Training loop, Gradient calculation

Gradient Descent is the fundamental tool used for optimizing the Loss Function.

When the `fit` method of a `Model` object is called

- it runs the *training loop* of Gradient Descent
- each iteration of the loop runs a *training step* of the `Model` on a mini-batch of training examples.

The default training step of a `Model`

- Runs the *forward* calculation:
    - presenting an input example to the NN inputs
    - calculating the NN outputs by Forward Propagation through the network
    - computing the Loss
    - computing the gradients of the Loss with respect to the NN weights
- Runs the *backward* calculation
    - propagating the Loss Gradient back from Loss Layer to Input layer via *Back Propagation*
    - updating the weights in the negative direction of the Gradient

Illustration of training loop

```
initialize(W)

# Training loop to implement mini-batch SGD
for epoch in range(n_epochs):`
    for X_batch, y_batch in next_batch(X_train, y_train, batch_size, shuffl
e=True):

        train_step(X_batch, y_batch)
```

Illustration of training step

```
# Training step: one iteration of the training loop
def train_step(X_batch, y_batch)
    # Forward pass
    y = NN(X_batch)

    # Loss calculation
    loss = loss_fn(y, y_batch)

    # Backward pass
    grads = gradient(loss, W)

    # Update
    W = W - grads * learning_rate
```

Let's explore the code for a training step in Keras.

- the `Model` object implements the default `training_step`
- here, we override it with our own implementation

Here is an example (from the notebook on [VAE (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/generative/ipynb/vae.ipynb)](https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/generative/ipynb/vae.ipynb) that we will study in depth in the future).

```
    def train_step(self, data):
        with tf.GradientTape() as tape:
            z_mean, z_log_var, z = self.encoder(data)
            reconstruction = self.decoder(z)
            reconstruction_loss = tf.reduce_mean(
                tf.reduce_sum(
                    keras.losses.binary_crossentropy(data, reconstruction), axi
s=(1, 2)
                )
            )
            kl_loss = -0.5 * (1 + z_log_var - tf.square(z_mean) - tf.exp(z_log_
var))
            kl_loss = tf.reduce_mean(tf.reduce_sum(kl_loss, axis=1))
            total_loss = reconstruction_loss + kl_loss
        grads = tape.gradient(total_loss, self.trainable_weights)
        self.optimizer.apply_gradients(zip(grads, self.trainable_weights))
        self.total_loss_tracker.update_state(total_loss)
        self.reconstruction_loss_tracker.update_state(reconstruction_loss)
        self.kl_loss_tracker.update_state(kl_loss)
        return {
```

In the above example, we override the default training step

- How to override a `Model`'s methods will be a future topic
- The mathematics of the VAE will be a future topic

For now, we focus on the code of the custom training step.

Note

We **didn't** create a `call` method for the `Model`

- we won't ever "call" the VAE model
    - only its `encoder` and `decoder` sub-components

Our training step

- calls the Encoder component using the batch `data` as input
- calls the Decoder component using the output of the Encoder
    - `reconstruction` is the approximation of `data`: reconstructed by the AutoEncoder
- computes a compound Loss (`total_loss`) consisting of two parts
    - `kl_loss`
    - `reconstruction_loss`
- calculates the Gradients
- applies the Gradients to update the weights

Let's focus on the computation of the Gradient of the Loss

- with respect to the model's weights (`self.trainable_weights`)

```
grads = tape.gradient(total_loss,
self.trainable_weights)
```

- In order to signal to TensorFlow that gradients are to be calculated for an expression
    - the expression must occur within the scope of a `tf.GradientTape` block

```
with tf.GradientTape() as tape:
```

We manually update the weights in the negative direction of the gradients

```
self.optimizer.apply_gradients(zip(grads,
self.trainable_weights))
```

We track the total loss as well as it's subparts

```
self.total_loss_tracker.update_state(total_loss)
        self.reconstruction_loss_tracker.update_state(reconstruction_loss)
        self.kl_loss_tracker.update_state(kl_loss)
```

We return 3 losses

```
return {
            "loss": self.total_loss_tracker.result(),
            "reconstruction_loss": self.reconstruction_loss_tracker.result(),
            "kl_loss": self.kl_loss_tracker.result(),
        }
```

Gradient Ascent

The calculation of gradients is powerful apart from deriving a model's weights.

TensorFlow allows you to compute the gradient of any expression with respect to any value on which the expression depends.

Let's visit this notebook on [Gradient Ascent (Gradient_ascent.ipynb)] to see how gradients can be used to visualize which inputs the various layers of a NN respond to most highly.

In [15]:

```
print("Done")
```

```
Done
```