Advanced Keras: motivation

We have been using the Keras Model API (mostly the Sequential) as a black box.

But it is highly customizable

- A Model is a class (as in Python object)
- It implements methods such as
 - compile
 - fit

We can change the behavior of a model in several ways

- Arguments to some methods are objects; we can pass non-default functions/objects
 - e.g., custom loss function
- We can override these (and other) methods to make our models do new things.

The Layer is also an abstract class (Python) in Keras.

Hence

- We can create new layer types
- We can override the methods of a given layer

In this module

- we will illustrate techniques that you can use to customize your Layers/Models.
- Illustrate the Functional model

Functional model: the basics, illustrated by the Transformer

The Sequential model

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

The Functional model

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

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)

There are actually 3 models in this <u>cell (https://colab.research.google.com/github/kerasteam/keras-</u>

<u>io/blob/master/examples/nlp/ipynb/neural_machine_translation_with_transformer.ipynb#s</u> we will visit!

Let's examine each one and try to relate the actual code to our picture.

pay close attention to the difference between \overline{y} (Encoder states) and y (Decoder outputs)

Transformer Layer (Encoder/Decoder)

In the above picture of the Transformer:

- ullet The output sequence $ar{\mathbf{y}}_{(1..ar{T})}$ (i.e., latent states) of the Encoder
 - Used in Decoder-Encoder attention
 - $||\bar{\mathbf{y}}|| = \bar{T} = \text{length of Transformer input}$
- ullet The prefix of the Decoder outputs generated up to time t
 - lacktriangle The Decoder output at time (t-1) is appended to the Decoder inputs available at time t
 - So the inputs are the Decoder outputs $\mathbf{y}_{(1..T)}$
 - $\circ T$ is full length of Transformer output
 - Causal (Masked) Attention is used to restrict the Decoder
 - $\circ~$ from attending at step t to any $\mathbf{y}_{(t)}$ where t>(t-1)
 - o Can't look at an output that hasn't been generated yet!

First model: the Encoder side of the Transformer

The Encoder side of the transformer:

```
encoder_inputs = keras.Input(shape=(None,), dtype="int64", name="encoder_input
s")
x = PositionalEmbedding(sequence_length, vocab_size, embed_dim)(encoder_inputs)
encoder_outputs = TransformerEncoder(embed_dim, latent_dim, num_heads)(x)
encoder = keras.Model(encoder_inputs, encoder_outputs)
```

This illustrates the pattern common to Functional models

- The output of a layer is assigned to a variable (e.g., encoder_inputs has the value of the model's inputs)
- The output of a layer is connected to the input of another layer via "function call" syntax
 - e.g., encoder_inputs is applied as the input to the PositionalEmbedding layer

x = PositionalEmbedding(sequence_length, vocab_size, embed_dim)
(encoder_inputs)

The collection (not necessarily a sequence) of Layer calls defines a graph of function calls that maps Model inputs to outputs.

To turn this collection into a Model

- We define which function to feed Model inputs to
- We define which function's outputs are the output of the model

For example, we define the Encoder side (sub-model of the Transformer) of the Transformer via

```
encoder = keras.Model(encoder_inputs, encoder_outputs)
```

This defines encoder to be a Model with

- input: Layer encoder_inputs (i.e., the Input layer)
- output: Layer encoder_outputs (i.e., the TransformerEncoder)

We can see the Encoder side in pictures via

```
tf.keras.utils.plot_model(
    encoder,
    show_shapes=True,
      encoder_inputs
                       input:
                               [(None, None)]
                                                [(None, None)]
        InputLayer
                      output:
  positional_embedding
                         input:
                                  (None, None)
                                                (None, None, 256)
  PositionalEmbedding
                        output:
transformer_encoder
                      input:
                              (None, None, 256)
                                                  (None, None, 256)
TransformerEncoder
                     output:
```

Encoder side of Transformer

Note: the input and output of a Model don't have to be Layer types!

There is also a model for the Decoder side of the Transformer in the cell we will visit:

```
decoder = keras.Model([decoder_inputs, encoded_seq_inputs], decoder_outputs)
```

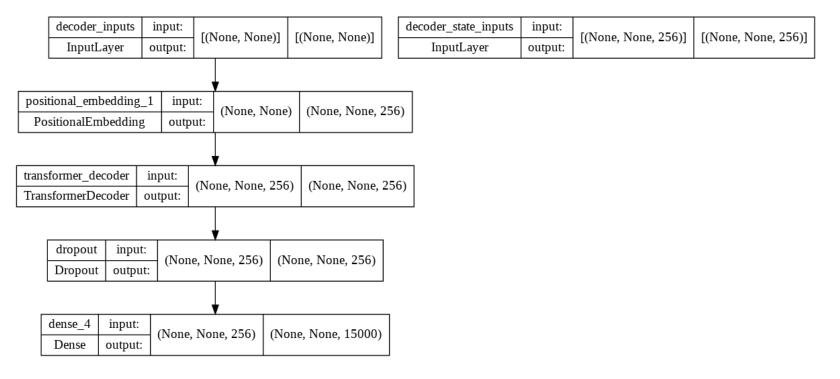
- input: An array of 2 Layer types -- [decoder_inputs, encoded_seq_inputs]
- output: Layer: decoder_outputs

Hence, the Decoder side takes a **pair** of inputs, as per the diagram.

decoder = keras.Model([decoder_inputs, encoded_seq_inputs], decoder_outputs)

Let's see if we can trace which role each element of the pair serves.

Here is picture of the Decoder side of the Transformer



Decoder side of Transformer

Note in the Decoder picture

```
decoder_state_inputs (on the right hand side) is assigned to variable
encoded_seq_inputs:
```

```
encoded_seq_inputs = keras.Input(shape=(None, embed_dim), name="decoder_state_i
nputs")
```

and encoded_seq_inputs is the second argument to TransformerDecoder

Hence, there should be an arrow from decoder_state_inputs to the transformer_decoder box.

This confirms that

- The Decoder sides takes a pair of inputs
- The second input is directed to the second argument of TransformerDecoder

Let's examine the Encoder code more closely

```
encoder_inputs = keras.Input(shape=(None,), dtype="int64", name="encoder_input
s")
x = PositionalEmbedding(sequence_length, vocab_size, embed_dim)(encoder_inputs)
encoder_outputs = TransformerEncoder(embed_dim, latent_dim, num_heads)(x)
encoder = keras.Model(encoder_inputs, encoder_outputs)
```

First, observe that the <code>Encoder</code> outputs ($ar{\mathbf{y}}_{(1..ar{T})}$) <code>encoder_outputs</code>

```
encoder = keras.Model(encoder_inputs, encoder_outputs)
```

We see that these Encoder outputs become the second part of the pair of the actual arguments that are the inputs to the *Decoder*

```
decoder_outputs = decoder([decoder_inputs, encoder_outputs])
```

And the formal argument of decoder definition is encoded_seq_inputs

```
decoder = keras.Model([decoder_inputs, encoded_seq_inputs], decoder_outputs)
```

So the encoder_outputs $(\bar{\mathbf{y}}_{(1..\bar{T})})$ become bound to encoded_seq_inputs within the Decoder.

Hence, the second part of the input pair of <code>decoder</code> serves the role of $\bar{\mathbf{y}}_{(1..\bar{T})}$, the sequence of Encoder latent states

Second model: The Decoder side of the Transformer

Now, let's look at the Decoder.

```
decoder_inputs = keras.Input(shape=(None,), dtype="int64", name="decoder_input
s")
encoded_seq_inputs = keras.Input(shape=(None, embed_dim), name="decoder_state_i
nputs")
x = PositionalEmbedding(sequence_length, vocab_size, embed_dim)(decoder_inputs)
x = TransformerDecoder(embed_dim, latent_dim, num_heads)(x, encoded_seq_inputs)
x = layers.Dropout(0.5)(x)
decoder_outputs = layers.Dense(vocab_size, activation="softmax")(x)
decoder = keras.Model([decoder_inputs, encoded_seq_inputs], decoder_outputs)
```

By tracing variable $\, {\sf x} \,$ backwards from the Decoder output (${f y}_{(1..T)}$) decoder_outputs

decoder_outputs = layers.Dense(vocab_size, activation="softmax")(x)

we can see the outputs derive from Layer sub-type TransformerDecoder

x = TransformerDecoder(embed_dim, latent_dim, num_heads)(x, encoded_seq_inputs)

We have already shown that $\, {f encoded_seq_inputs} \, \, {f corresponds} \, {f to} \, {f ar y}_{(1..ar T)} \,$

So we can guess that variable $\, {\bf x} \,$ in the call to $\, {\bf Transformer Decoder} \,$ corresponds to $\, {\bf y}_{(1..T)} \,$

Let's confirm that.

Tracing variable x backwards from its use a the first argument in the TransformerDecoder

x = PositionalEmbedding(sequence_length, vocab_size, embed_dim)(decoder_inputs)

we see that it is the positionally-encoded (to enable Causal masking) decoder_inputs

- The Positional Embedding is added to enforce Masking (causal ordering)
 Hopefully: decoder inputs are the decoder outputs shifted by one time step
 - That is: the training set enforces "Teacher Forcing"

Third model: the full Transformer – Encoder + Decoder

Finally, there is the Transformer Model, combining an Encoder and Decoder:

```
decoder_outputs = decoder([decoder_inputs, encoder_outputs])
transformer = keras.Model(
    [encoder_inputs, decoder_inputs], decoder_outputs, name="transformer")
```

The transformer input is a pair

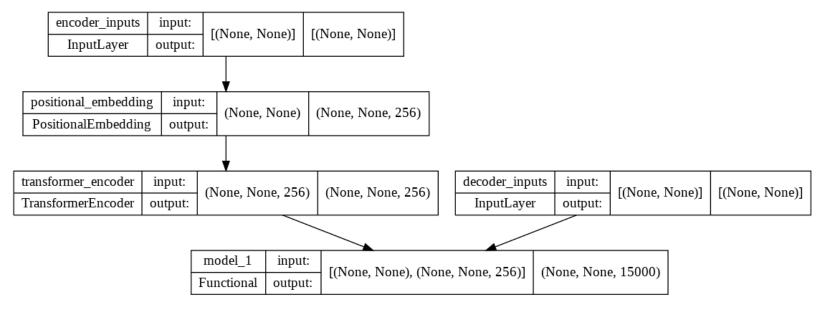
[encoder_inputs, decoder_inputs]

And it's output is

decoder_outputs

We identify the first part of the input pair (<code>encoder_inputs</code>) as the input sequence $\mathbf{x}_{(1\dots ar{T})}$

Here is the picture of the full Transformer:



Full Transformer

Note: Where does "Teacher Forcing" happen?

We had "hoped" that

decoder_inputs are the decoder_outputs shifted by
one time step

- which needs to be true at training time to implement "teacher forcing"
- (but which shouldn't happen at inference time)

Where in the code does this happen?

In the data preparation, we can see that each row of the training data is mapped by the function

```
def format_dataset(eng, spa):
    eng = eng_vectorization(eng)
    spa = spa_vectorization(spa)
    return ({"encoder_inputs": eng, "decoder_inputs": spa[:, :-1],}, spa[:,
1:])
```

where eng is $\mathbf{x}_{1\ldots ar{T}}$ and spa is $\mathbf{y}_{1\ldots T}$

The function replaces the ("feature", "target") example pairs

• denoted as (eng, spa) in the code (n.b., the "feature" is a sentence in English; the "target" a sentence in Spanish)

by

- example features are the hash ({"encoder_inputs": eng, "decoder_inputs": spa[:, :-1],},
- example target is now spa[:, 1:]

So decoder_inputs would seem to be the un-shifted sequence of words in the Spanish sentence.

But wait!

Careful examination of the Spanish sentences show that they begin with a [start] token

- This, in essence, has shifted the decoder_input by one word
- So the first output of the Decoder will be the first (non-[start]) word of Spanish
- Which will be compared to the new target spa[:, 1:], which is the first (non-[start]) word of Spanish

At inference time, we do not see Teacher Forcing:

We can see the generated output decoded_sentence built up one word at a time in the code snippet for decode_sequence

```
def decode_sequence(input_sentence):
    tokenized_input_sentence = eng_vectorization([input_sentence])
    decoded_sentence = "[start]"
    for i in range(max_decoded_sentence_length):
        tokenized_target_sentence = spa_vectorization([decoded_sentence])[:, :-

1]
    predictions = transformer([tokenized_input_sentence, tokenized_target_s
entence])
    ....

    decoded_sentence += " " + sampled_token

    if sampled_token == "[end]":
        break
    return decoded_sentence
```

Summary

A lot going on here!

- A complex connection of Layer outputs to inputs
- Custom Layer sub-types
 - PositionalEmbedding, TransformerEncoder, TransformerDecoder
 - We will soon see how to define our own Layer sub-classes
- Teacher Forcing

That concludes our first look at the Functional model

Model specialization

Custom loss (passing in a loss function)

In introducing Deep Learning, we have asserted that

It's all about the Loss function

That is: the key to solving many Deep Learning problems

- Is not in devising a complex network architecture
- But in writing a Loss function that captures the semantics of the problem

Up until now

- We have been using pre-defined Loss functions (e.g., binary_crossentropy)
- Specifying the Loss function in the compile statement

model.compile(loss='binary_crossentropy')

You can write your own loss functions (https://keras.io/api/losses/)

In Keras, a Loss function has the signature

loss_fn(y_true, y_pred, sample_weight=None)

Custom train step (override train_step)

But what if your Loss function needs access to values that are not part of the signature?

Or what if you want to change the training loop?

You could write your own training loop by overriding the fit method

- Cycle through epochs
- Within each epoch, cycle through mini-batches of examples
- For each mini-batch of examples: execute the train step
 - forward pass: feed input examples to Input layer, obtain output
 - compute the loss
 - Compute the gradient of the loss with respect to the weights
 - Update the weights

Rather than overriding fit, it sometimes suffices to override the train step: train_step

Let's start by looking at the "standard" implementation of a basic train step.

We will see

- How losses are computed
- Gradients are obtained
- Weights are updated

Basic train_step

(https://colab.research.google.com/github/tensorflow/docs/blob/snapshotkeras/site/en/guide/keras/customizing what happens in fit.ipynb#scrollTo=9022333acaa We can modify the basic training step too.

For example: suppose we want to make some training examples "more important" than others

- Rather than Total Loss as equally-weighted average over all examples
- Pass in per-example weights

This might be useful, for example, when dealing with Imbalanced Data

Layer specialization

A Layer in Keras is an abstract (Python) object

- instantiating the object returns a function
 - That maps input to the layer to the output

We have used specific instances of Layer objects (e.g., Dense) as arguments in the list passed to the Sequential model type.

We can also use instances in the Functional Model.

For example

- Dense(10)
 - Is the constructor for a fully connected layer instance with 10 units
 - The constructor returns a function
 - The the function maps the layer inputs to the outputs of the computation defined by the layer

So you will see code fragments like > x = Input(shape=(784)) x = Dense(10, activation=softmax)(x)

• Re-using the variable x as the output of the current layer

When the function is invoked, the Layer's call method is used

- call gets invoked implicitly by "parenthesized argument" juxtaposition
 - e.g., Dense(10) (x)
 - is similar to obj=Dense(10); result = obj.call(x)`
- The function maps the inputs to the layer to the output

Overriding call allows us to defined a new Layer sub-class.

For example, https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/nlp/ipynb/neural machine translation with transformer.ipynb#s is the code defining some new Layer types that will be used to create a Transformer layer type.

The output of Dense(10) is a Tensor with final dimension equal to the number of units (e.g., 10)

- The Tensor has leading dimensions too
 - e.g., the implicit "batch index" dimension
 - since the layer takes a mini-batch of examples (rather than a single example) as input
- It may have additional dimensions too!
 - Just like numpy: threading over additional dimensions
 - e.g., if input is shape (minibatch_size \times $n_1 \times n_2$)
 - \circ output is shape (minibatch_size \times $n_1 \times 10$)
 - Dense operates over the final dimension

Studying advanced models

The best way to learn is to study the code of some non-trivial models

Transformer: Custom layers, Skip connections, Layer Norm

We have already seen part of the Transformer in introducing the basics of the Functional model.

We use the rest of this example to discover other advanced Keras techniques:

<u>Transformer layer (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/nlp/ipynb/neural_machine_translation_with_transformer.ipynb#sIMkSs)</u>

- <u>Custom layers (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/nlp/ipynb/neural_machine_translation_with_transformer.i</u>
- Layer Norm
- Skip connections

Custom layers: subtle point

Let's look at the constructor for the TransformerEncoder custom layer, as an example

The custom layer consists of a collection of component layers

Why are the components layers (e.g., Dense, MultiHeadAttention, LayerNormalization) instantiated in the class constructor

As opposed to being defined in the call method

Had we instantiated each component within the call method

- There would be a new instance of each component each time the layer was called on an example in training!
- Each instance would have it's own weights
- So training would not "learn" between examples

Other custom layers of interest

We can dig deeper to examine how the Attention layers are implemented in code:

- <u>Scaled dot-product attention</u>
 <u>(https://www.tensorflow.org/text/tutorials/transformer#scaled dot_product_attention)</u>
- <u>Multi-head attention (https://www.tensorflow.org/text/tutorials/transformer#mult head attention)</u>

VAE: Custom Model – Training Loop, the Gradient Tape

<u>Variational Autoencoder (VAE) from github</u> (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/generative/ipynb/vae.ipynb#scrollTo=DEU05Oe0vJrY)

 VAE: Custom train step (https://colab.research.google.com/github/kerasteam/kerasio/blob/master/examples/generative/ipynb/vae.ipynb#scrollTo=0EHkZ1WCHw9E)

Complex loss

We use this example to illustrate

- How to sub-class the Model abstract class
- How to create a custom training loop
 - the "Gradient tape"

Issues

- Custom model (not layer) class VAE
- The reconstruction loss depends on the output of the Decoder part of the VAE
 - No other obvious way to define this loss aside from a custom training step
- Because we are computing the Loss in the training step
 - we must compute the gradient of the Loss w.r.t weights
 - Update the weights (gradient tape)

Visualizing what CNN's learn: Gradient Ascent and the Gradient Tape

<u>Visualizing what Convnets learn (https://colab.research.google.com/github/kerasteam/keras-</u>

io/blob/master/examples/vision/ipynb/visualizing_what_convnets_learn.ipynb#scrollTo=K

- The Gradient Tape
- Maximize utility (negative loss)
 - mean (across the spatial dimensions) of one feature map in a multi-layer
 CNN
 - the "weights" being solved for are the pixels of the input image!

We use this example to show how powerful the Gradient Tape is

<u>Gradient ascent (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/vision/ipynb/visualizing what convnets learn.ipynb#scrollTo=a9</u>

Factor Models and Autoencoders: Threading

We use this example to show

- A Functional model applied to a common problem in Finance.
- Threading

We will cover the Finance aspects of this in a <u>separate module</u> (<u>Autoencoder for conditional risk factors.ipynb</u>)

For now, I want to focus on the idea and the code

Here is the code, excerpted from the <u>notebook (https://github.com/stefan-jansen/machine-learning-for-trading/blob/main/20</u> autoencoders for conditional risk factors/06 conditional autoencoders

```
def make_model(hidden_units=8, n_factors=3):
    input_beta = Input((n_tickers, n_characteristics), name='input_beta')
    input_factor = Input((n_tickers,), name='input_factor')

    hidden_layer = Dense(units=hidden_units, activation='relu', name='hidden_la
yer')(input_beta)
    batch_norm = BatchNormalization(name='batch_norm')(hidden_layer)

    output_beta = Dense(units=n_factors, name='output_beta')(batch_norm)

    output_factor = Dense(units=n_factors, name='output_factor')(input_factor)

    output = Dot(axes=(2,1), name='output_layer')([output_beta, output_factor])

    model = Model(inputs=[input_beta, input_factor], outputs=output)
    model.compile(loss='mse', optimizer='adam')
    return model
```

Not obvious what is going on here.

A picture will help:

Autoencoder for Conditional Risk Factors

Threading

Let's focus on the Dense layer corresponding to the box labelled "Beta" in the picture

ullet Dense $(n_{
m factors})$

From the diagram you will notice that

- ullet the input to this layer is *two dimensional*: $(n_{
 m tickers} imes n_{
 m chars})$
- ullet the output to this is *two dimensional*: $(n_{
 m tickers} imes n_{
 m factors})$

We have not yet seen multi-dimensional input/output in regard to a Dense layer

What is going on here?

The layer is implementing a function with signature

```
egin{aligned} \bullet \; \mathsf{Dense}(n_{\mathrm{factors}}) \ & dots \ (n_{\mathrm{tickers}} \ & 	imes n_{\mathrm{chars}}) \ & dots \ (n_{\mathrm{tickers}} \ & 	imes n_{\mathrm{factors}}) \end{aligned}
```

Tensorflow/Keras works on higher dimensional objects just like NumPy:

threading (https://www.tensorflow.org/api docs/python/tf/keras/layers/Dense)
 over "extra" dimensions

If the input to layer l is shape $(d_{(l),1} imes d_{(l),2} imes \dots d_{(l),N} imes n_{(l)})$

- And the layer type operates over a *single* dimension (usually the last dimension)
 - lacksquare producing output shape $n_{(l+1)}$

Then threading treats the inputs

In our case

- Input shape is $(n_{ ext{tickers}} imes n_{ ext{chars}})$
- ullet The Dense layer is defined with $n_{
 m factors}$ units ($n_{(l+1)}=n_{
 m factors}$)
- ullet Hence, the output shape is $(n_{
 m tickers} imes n_{
 m factors})$

The weight matrix for this layer

- ullet \mathbf{W}_eta with shape $(n_{ ext{factors}} imes n_{ ext{chars}})$
 - just like any Dense layer; number of weights is independent of threading
- ullet applies the *same weights* to each of the $n_{
 m tickers}$ (the rows) of the input

Neural Style Transfer: Feature extractor, Training Loop

We use this example to illustrate

- <u>Complex Loss and Training Loop</u>
 (https://keras.io/examples/generative/neural style transfer/#compute-the-style-transfer-loss)
- <u>Feature extractor</u>
 (https://keras.io/examples/generative/neural-style-transfer-#compute-the-style-transfer-loss)

<u>Here (https://www.tensorflow.org/tutorials/generative/style_transfer)</u> is a tutorial view of the notebook.

Autoencoder: Functional model

<u>Autoencoder example from github (https://colab.research.google.com/github/kenperry-public/ML_Spring_2022/blob/master/Autoencoder_example.ipynb)</u>

Functional model

Issues

- We could use a Sequential model with initial Encoder layers and final Decoder layers
 - But we would not be able to independently access the Encoder nor the Decoder as isolated models

GAN

Simple GAN (https://keras.io/examples/generative/dcgan_overriding_train_step)

<u>Custom train step: GAN training</u>
 (https://keras.io/examples/generative/dcgan overriding train step/#override-trainstep)

Wasserstein GAN with Gradient Penalty

Wasserstein GAN with Gradient Penalty (https://keras.io/examples/generative/wgan_gp/#create-the-wgangp-model)

- <u>Gradient Tape: used for loss term, rather than weight update</u> (https://keras.io/examples/generative/wgan_gp/#create-the-wgangp-model)
- Overide compile (https://keras.io/examples/generative/wgan_gp/#create-the-wgangp-model)
- <u>Custom train step: GAN training</u>
 <u>(https://keras.io/examples/generative/wgan_gp/#create-the-wgangp-model)</u>

```
In [2]: print("Done")
```

Done