





For AOS551 Fall 2021 Deep Learning in Geophysical Fluid Dynamics Ming-Ruey (Ray) Chou

LEARNING RESOURCES

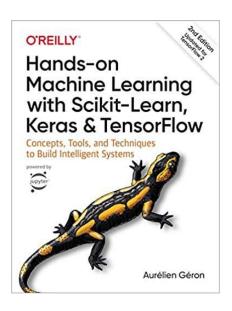


Guide and Tutorial

Great explanation, detailed and thorough

Simply too much, hard to get started (need hours of reading)

Focus on traditional deep learning (CV, NLP, RL), which may not suit our needs



Very hands-on, thus lack some key details.

Suitable as a starter, but after which one still needs the official site.

(Comments are for the 1st edition)

TOPICS COVERED

TENSOR	NumPy Array, Tensor, Variable	
AND ITS OPERATION	Taking Gradients	
BUILDING A MODEL	Raw Variables or Keras Create/Save/Load Weights	
INTERGRATE	Data loading Training loop	
TIPS & PITFALLS	Debugging tips Optimization tips	



TOPICS **NOT** COVERED

Eager execution/Graph Execution, or TensorFlow 2.X/TensorFlow 1.X

Stick to 2.X, until training speed bothers you Graphs and tf.function explained by official site

tf.data.Dataset API

Use something simple, except large (>> 10G) data. Input pipelines explained by official site

Certain Useful but Baffling Keras API

model.fit, mode.compile, Callbacks, Functional API, .etc.

For simple models and training steps, the time to learn these does not justify

Keras explained by official site



NUMPY ARRAY

```
ARRAY CREATION
                                             ARRAY PROPERTIES
                                          In [4]: arr.dtype
In [1]: import numpy as np
                                          Out[4]: dtype('int64')
In [2]: arr = np.array(
   ...: [[1, 2, 3], [4, 5, 6]]
                                          In [5]: ones.dtype
   . . . : )
                                          Out[5]: dtype('float64')
In [3]: arr
                                          In [6]: arr.shape
Out[3]:
                                          Out[6]: (2, 3)
array([[1, 2, 3],
       [4, 5, 6]]
                                          In [7]: ones.shape
                                          Out[7]: (3, 4)
In [4]: ones = np.ones((3, 4))
                                          In [8]: arr.size
In [5]: ones
                                          Out[8]: 6
Out[5]:
array([[1., 1., 1., 1.],
                                          In [9]: ones.size
       [1., 1., 1., 1.]
                                          Out[9]: 12
       [1., 1., 1., 1.]])
```



NUMPY ARRAY

ARITHMETIC OPERATIONS

SLICING



TENSORFLOW TENSOR

```
In [1]: import tensorflow as tf
In [3]: ts = tf.constant(
   ...: [[1, 2, 3], [4, 5, 6]]
   ...: )
In [4]: ts
Out[4]:
<tf.Tensor: shape=(2, 3), dtype=int32, numpy=
array([[1, 2, 3],
       [4, 5, 6], dtype=int32)>
In [5]: ts ones = tf.ones((3, 4), dtype=tf.float32)
In [6]: ts ones
Out[6]:
<tf.Tensor: shape=(3, 4), dtype=float32, numpy=
array([[1., 1., 1., 1.],
       [1., 1., 1., 1.],
       [1., 1., 1., 1.]], dtype=float32)>
```

TENSOR CREATION

TENSOR PROPERTIES In [7]: ts.dtype Out[7]: tf.int32 In [8]: ts ones.dtype Out[8]: tf.float32 In [9]: ts.shape Out[9]: TensorShape([2, 3]) In [10]: ts ones.shape Out[10]: TensorShape([3, 4]) In [11]: tf.size(ts) Out[11]: <tf.Tensor: shape=(), dtype=int32, numpy=6> In [12]: tf.size(ts ones) Out[12]: <tf.Tensor: shape=(),</pre> dtype=int32, numpy=12>

TENSOR AND ITS OPERATION

TENSORFLOW TENSOR

```
ARITHMETIC OPERATIONS
                                                               SLICING
                                                    In [27]: ts[0, 0]
In [19]: ts * 10
                                                    Out[27]: <tf.Tensor: shape=(),</pre>
Out[19]:
<tf.Tensor: shape=(2, 3), dtype=int32, numpy=
                                                              dtype=int32, numpy=1>
array([[10, 20, 30],
       [40, 50, 60]], dtype=int32)>
                                                    In [28]: ts[0, :]
                                                    Out[28]: <tf.Tensor: shape=(3,),
In [20]: ts ** 2
                                                               dtype=int32, numpy=array([
Out[20]:
                                                               1, 2, 3], dtype=int32)>
<tf.Tensor: shape=(2, 3), dtype=int32, numpy=
array([[1, 4, 9],
       [16, 25, 36]], dtype=int32)>
                                                    In [30]: ts[:, 1:3]
                                                    Out[30]:
In [21]: tf.matmul(
                                                    <tf.Tensor: shape=(2, 2), dtype=int3
    ...: ts, tf.cast(ts ones, dtype=tf.int32)
                                                    array([[2, 3],
    . . . : )
                                                            [5, 6]], dtype=int32)>
Out[21]:
<tf.Tensor: shape=(2, 4), dtype=int32, numpy=
array([[ 6, 6, 6, 6],
       [15, 15, 15, 15], dtype=int32)>
```

TENSOR AND ITS OPERATION

Array – Tensor Operations

TENSOR/NUMPY ESSENTIALS

Explicit conversion (via .numpy() / tf.constant)

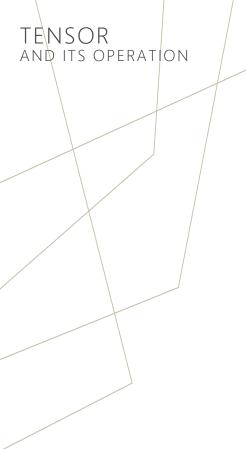
Automatic conversion (sometimes)

Tensor/NumPy API Similarity

One could expect, at least for the basic NumPy ndarray operations, TensorFlow provides similar syntax or functionality

However, aiming for parallel computing makes some fundamental differences between the two (similar operations still included, but wonkier and less computationally efficient)

We cover some important differences between them in next slides



Array-Like, but Strict Type

Array, Automatic Type Conversion:

Note: dtype of arr is int64, ones is float64

Tensor Operation is Strict Type

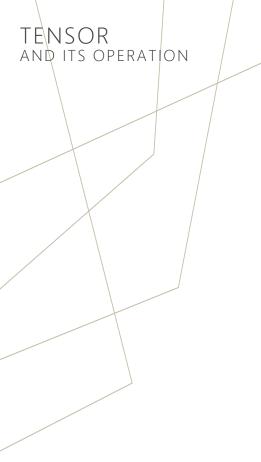
```
In [29]: ts * ts_ones[0:2, 0:3]
```

InvalidArgumentError:

cannot compute Mul as input #1(zero-based) was expected to be an int32 tensor but is a float tensor [Op:Mul]

TENSOR/NUMPY ESSENTIALS

Need to Cast Datatype before Operations:



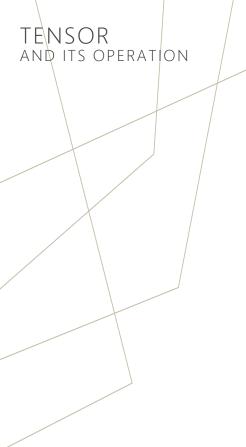
TENSOR/NUMPY ESSENTIALS

but **Hard for Advanced Slicing**

Advanced Slicing for Array:

Results in Error for Tensor

Can achieve similar operation in TensorFlow, but cumbersome.



but Immutable for 'normal' Tensor

Change Value(s) in Array

Results in Error for Tensor

In
$$[33]$$
: $ts[0, 0] = 10$

TypeError:

'tensorflow.python.framework.ops.EagerTensor' object does not support item assignment

TENSOR/NUMPY ESSENTIALS

Tensor in general is immutable.

The only way to change values in existing Tensor is to use *Variable*.

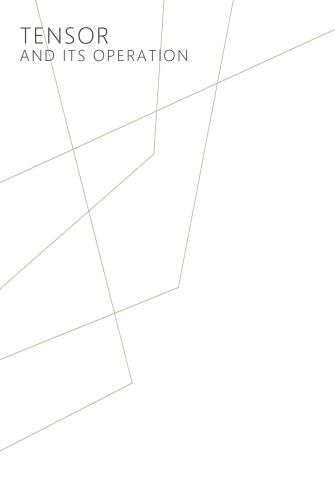


VARIABLE, Tensor whose values are modifiable

IS A TENSOR

WITH METHOD TO CHANGE ITS VALUES

REMARK - Model weights are Variables



REMARKS **KISS** (**K**eep **i**t **s**imple, **s**tupid)

- Do explicit conversion instead of automatic
- Stick to dumb simple operations
- Broadcasting is powerful but leads to obscure bugs. Keep dimension and shape as simple as possible (while considering batch dimension)

TENSOR/NUMPY ESSENTIALS

What is broadcast? General rule for NumPy array operation Array (elementwise) Multiply:

```
A (4d array): 8 x 1 x 6 x 1
B (3d array): 7 x 1 x 5
Result (4d array): 8 x 7 x 6 x 5
```

From NumPy official site

```
x = tf.Variable(3.0)
with tf.GradientTape() as tape:
  y = x**2

Roughly equals:
  tape = tf.GradientTape()
  tape.__enter__()
```

```
# dy = 2x * dx
dy_dx = tape.gradient(y, x)
dy_dx.numpy()
```

>>> will get 6.0

The GradientTape is the fundamental tool in TensorFlow to do automatic differentiation (i.e., calculate gradient)

To understand how automatic differentiation works, see:

```
[dl_dw, dl_db] = tape.gradient(loss, [w, b])
[dy_dw, dy_db] = tape.gradient(y, [w, b])
```

Use the same tape to get gradient second time won't work without being persistent

```
# A trainable variable
x0 = tf.Variable(3.0, name='x0')
# Not trainable
x1 = tf.Variable(3.0, name='x1', trainable=False)
# Not a Variable: A variable + tensor returns a tensor.
x2 = tf.Variable(2.0, name='x2') + 1.0
# Not a variable
x3 = tf.constant(3.0, name='x3')
with tf.GradientTape() as tape:
  v = (x0**2) + (x1**2) + (x2**2)
grad = tape.gradient(y, [x0, x1, x2, x3])
for q in grad:
  print(g)
```

Yield proper gradients only for x0

```
tf.Tensor(6.0, shape=(), dtype=float32)
None
None
None
```

GradientTape traces only **trainable Variables** by default

```
Note:
x1 is not-trainable
x2 is a Tensor! (The addition +1.0 returns a Tensor)
```



Explicit stated which Tensor/Variable you want to get derivatives

```
x = tf.constant(3.0)
with tf.GradientTape() as tape:
   tape.watch(x)
   y = x**2

# dy = 2x * dx
dy_dx = tape.gradient(y, x)
print(dy_dx.numpy())
```

>>> will get 6.0

All the parameters along the way are traced, so we can get derivative w.r.t to intermediate result

```
x = tf.constant(3.0)
with tf.GradientTape() as tape:
   tape.watch(x)
   y = x * x
   z = y * y

# Use the tape to compute the gradient of z with
# intermediate value y.
# dz_dy = 2 * y and y = x ** 2 = 9
print(tape.gradient(z, y).numpy())
```



TAKE GRADIENT AND UPDATE

Simple Gradient Descent example: manually calculating the gradients and updating the values

```
with tf.GradientTape() as t:
    # Trainable variables are automatically tracked by GradientTape
    current_loss = loss(y, model(x))

# Use GradientTape to calculate the gradients with respect to W and b
dw, db = t.gradient(current_loss, [model.w, model.b])

# Subtract the gradient scaled by the learning rate
model.w.assign_sub(learning_rate * dw)
model.b.assign_sub(learning_rate * db)
```



TAKE GRADIENT AND UPDATE, USING BUILT-IN OPTIMIZERS

apply_gradients wraps all the calls required for updating weights, also the calculation for learning rate .etc.

```
adam = tf.keras.optimizers.Adam(learning_rate=0.01)
with tf.GradientTape() as tape:
    losses = loss(y, model(x))

gradients = tape.gradient(losses, model.trainable_variables)
adam.apply_gradients(zip(gradients, model.trainable_variables))
```

KERAS INTERFACE

It wraps the Tensor/Variable as realization of high level concepts such us layers, weight initialization, model, optimizer .etc

Working in high-level concept is time saving and less error-prone

LAYERS & MODELS IN KERAS

CREATE A LAYER

It's a fully-connected layer of 50 nodes with tangent hyperbolic activation

```
input_layer = InputLayer(input_shape=(1,))
```

InputLayer is a specialized layer without any weights & activation

It just determine the dimension of the input data (1D input in this case)

STACK LAYERS TO MODEL

REMARK – Check the tf.keras.layers module most of the commonly used operations are already there

LAYERS & MODELS IN KERAS

THE STRUCTURE OF MODEL

model.summary() display the structure of the neural network

Layer (type)	Output	Shape	Param #
dense (Dense) dense_1 (Dense)	(None,	•	100 51
Total params: 151 Trainable params: 151 Non-trainable params: 0			

FORWARD-PASS

REMARK - the *batch dimension* is automatically taking care of, which reduces much trouble.

LAYERS & MODELS IN KERAS

FORWARD-PASS 2D EXAMPLE

```
Specify your input as 2D, so the model
model = keras.Sequential()
                                            expects the input shape to be (batch, 2)
model.add(InputLayer(input_shape=(2,)))
model.add(Dense(50))
model.add(Dense(3))
                                                                    Output Shape
                                                     Layer (type)
                                                                                  Param #
model.summary()
                                                     dense (Dense)
                                                                     (None, 50)
                                                                                  150
                                                                     (None, 3)
                                                     dense 1 (Dense)
# output is a Tensor with shape (100, 3)
points = tf.ones((100, 2))
                                                     Total params: 303
                                                     Trainable params: 303
outputs = model(points)
                                                     Non-trainable params: 0
\# u, v, h are with shape (100,)
velocity u = outputs[:, 0]
                                    Model output shape is (batch, 3)
velocity v = outputs[:, 1]
                                    Slice the (stacked) model outputs to get the separate component
hardness h = outputs[:, 2]
                                    of your physical system
```

RAW TENSOR OPERATIONS Versus KERAS MODEL BUILDING

Using Raw Tensors/Variables

```
class MyNet:
   def init (self):
       layers = [1, 50, 50, 50, 1]
       # initialize weights and biases
       initializer = tf.keras.initializers.GlorotNormal()
       self.weights = []
       self.biases = []
       for 1 in range(len(layers) - 1):
           W = initializer(shape=(layers[1], layers[1 + 1]))
           b = tf.Variable(tf.zeros([1, layers[l + 1]], dtype=tf.float32))
           self.weights.append(W)
           self.biases.append(b)
       self.trainable variables = self.weights + self.biases
   def forward(self, x):
       H = x
       for l in range(len(self.weights) - 1):
           W = self.weights[1]
           b = self.biases[1]
           H = tf.tanh(tf.add(tf.matmul(H, W), b))
       W = self.weights[-1]
       b = self.biases[-1]
       Y = tf.add(tf.matmul(H, W), b)
       return Y
```

Using Keras

```
model = keras.Sequential()
model.add(InputLayer(input_shape=(1,)))
model.add(
    Dense(50, activation="tanh",
        dtype=tf.float32,
        kernel initializer="glorot normal"))
model.add(
    Dense(50, activation="tanh",
        dtype=tf.float32,
        kernel initializer="glorot normal"))
model.add(
    Dense(50, activation="tanh",
        dtype=tf.float32,
        kernel initializer="glorot normal"))
model.add(
    Dense(1, activation="tanh",
        dtype=tf.float32,
        kernel initializer="glorot normal"))
model.summary()
```

USING KERAS MODEL

WEIGHTS CREATED AUTOMATICALLY

Get a list of all trainable weights via model.trainable_variables, which is useful for updating weights

```
In [4]: model.trainable_variables
```

USING KERAS MODEL

UPDATE VARIABLES

```
adam = tf.keras.optimizers.Adam(learning_rate=0.01)
with tf.GradientTape() as tape:
    losses = loss(y, model(x))

gradients = tape.gradient(losses, model.trainable_variables)
adam.apply_gradients(zip(gradients, model.trainable_variables))
```

SAVE/LOAD WEIGHTS

```
model.save_weights("my_model.h5")

# You have to recreate a model with EXACT same structure
model.load_weights("my_model.h5")
```

CAVEAT – load_weights with different model structure may silently fail, without any apparent warning/exception

OTHER CUSTOMIZABLE

CUSTOM LAYERS

CUSTOM INTIALIZER

```
class ExampleRandomNormal(tf.keras.initializers.Initializer):

def __init__(self, mean, stddev):
    self.mean = mean
    self.stddev = stddev

def __call__(self, shape, dtype=None, **kwargs):
    return tf.random.normal(
        shape, mean=self.mean, stddev=self.stddev, dtype=dtype)

def get_config(self): # To support serialization
    return {"mean": self.mean, "stddev": self.stddev}
```

EVEN CUSTOM OPTIMIZER! ...though harder

REMARKS - usually not needed, but can be useful sometimes

Also, checkout this wonderful colab demonstration

https://colab.research.google.com/drive/17u-pRZJnKN0gO5XZmq8n5A2bKGrfKEUg#scrollTo=UHOOlixcQ9Gl

INTERGRATE EVERYTHING Pseudo code demonstrates the fundamental elements of a training script x_data, y_data = ... # get your data model = ... # create model opt = ... # Use built-in optimizer for iteration in range(...): with **tf.GradientTape**() as tp: prediction = model(x_data) loss = MSE(y_data, prediction) weights = model.trainable_variabels grads = tp.gradient(loss, weights) opt.apply_gradients(zip(grads, weights))

```
def prepare_data():
     x_data, y_data = LOAD("data.mat")
     x data /= XSCALE
    y data /= YSCALE
    x data = x data[..., np.newaxis]
    y data = y data[..., np.newaxis]
    x tensor = tf.consant(x data)
    y tensor = tf.consant(y data)
     return x tensor, y tensor
x data, y data = ... # get your data
model = ... # create model
opt = ... # Use built-in optimizer
for iteration in range(...):
   with tf.GradientTape() as tp:
       prediction = model(x data)
       loss = MSE(y data, prediction)
   weights = model.trainable variabels
   grads = tp.gradient(loss, weights)
   opt.apply gradients(zip(grads, weights))
  INTERGRADE EVERYTHING
```

DATA LOADING

- a. Load
- b. Normalize
- c. Correct the Shape (First dimension is batch!)
- d. (Optional) Sample Data in Loop

When Data Fits Into Memory

Load entire data into memory before the training loop. Can choose to sample a subset at each iteration

```
random_shuffle(x_data, y_data)
for iteration in range(...):
    start = (iteration % 100) * 1000
    end = start + 999
    x_sampled = x_data[start:end, :]
    y_sampled = y_data[start:end, :]
    ...
```

When Dataset Is Large

Harder! Create an iterator over the model, fetch the data on the fly. Checkout input pipelines explained by official site

```
def equation loss(x, model):
    with tf.GradientTape(persistent=True) as tp:
         tp.watch(x)
         outputs = model(x)
         u = outputs[..., 0]
         v = outputs[..., 1]
    u x = tp.gradient(u, x)
    v x = tp.gradient(v, x)
    # Residues of Govering Equations
    equation = ALPHA * u x - BETA * v x
    return tf.reduce mean(equation ** 2)
x data, y data = ... # get your data
model = ... # create model
opt = ... # Use built-in optimizer
for iteration in range(...):
   with tf.GradientTape() as tp:
       prediction = model(x data)
       loss = MSE(y_data, prediction)
   weights = model.trainable variabels
   grads = tp.gradient(loss, weights)
   opt.apply gradients(zip(grads, weights))
 INTERGRADE EVERYTHING
```

OPTIMIZATION STEPS

- a. Calculate Loss
- b. Calculate Gradients
- c. Update Variables
- d. Display/Save for Monitoring

Monitor Is A Must

Loss values on train/validation set for every n iterations Include any relevant metrics

Store Intermediate Models Is Helpful

Robust against unexpected interruption

Easiest way to select model based on validation set

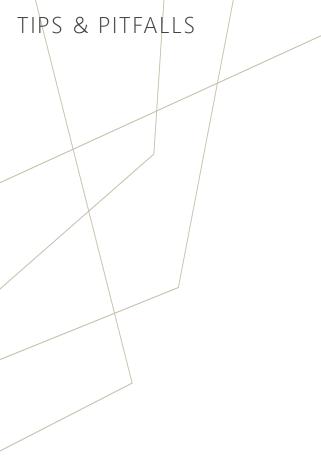
```
for iteration in range(...):
    ...

if iteration % 100 == 0:
    print(loss.numpy())
    model.save(f"at_it={iteration}.h5")
```

General Principle of Coding:

Keep Steps Small And Separated

- Debugging effort determined (almost solely) by suspected area
- Splitting code into different files helps
- Create small and simple functions you are confident with, and rely on them
- ❖ Able to revert to the previous working vesion (version control tool is helpful)



Use Simple .py file Instead of Notebook

Notebook remembers variable value even the cell is deleted or changed

The execution order may affect the result

Not suitable as scheduled job on cluster

Split Training and Plotting Code

Do NOT use an end-to-end code file for everything. Split, split!

Training and store the model using a stand-alone .py file

Load the stored model in another file to examination the result

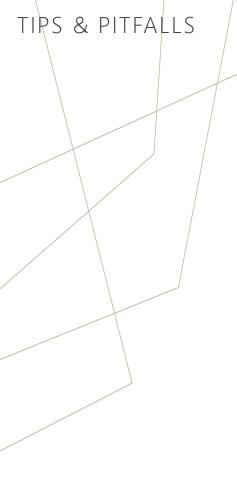
Start with Simplified Case as Sanity Check

Deep learning, especially the optimization, is hard to reason about

Ground project on simplified situation which we have clear expected result

Develop toward complex and long-running

MODEL TRAINING PITFALLS



Checklist When Model Performs Unreasonably Poor

- Have some simplified case that works as sanity check
- Does the model do the right calculation?
 - Careful on the numerical range of activation function
 e.g., tanh only outputs in [-1, 1]
 - Check the shape of input and output for each layer
- Is the long-term trend of loss curve decreasing?
 - Does the model weights change at all?
 - Try difference learning rates
 - Try different initializers

MODEL TRAINING PITFALLS

- Are the loss values sane?
- Learn from the Model Prediction
 - In which domain, it performs poorly?
 - Is there any patterns in the prediction?



ENJOY, GOOD LUCK

REACH FOR HELP

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Office hour: Tuesday 13:00 - 14:00

- AMA via email/canvas
- Other slots are available via appointment