Introduction to gradients and automatic differentiation

Run in Google Colab (https://colab.research.google.com/github/tensorflow/docs/blob/master/site/en/guide/autodiff.ipynb) | View source on GitHub (http

Automatic Differentiation and Gradients

Automatic differentiation (https://en.wikipedia.org/wiki/Automatic_differentiation) is useful for implementing machine learning algorithms such as backpropagation (https://en.wikipedia.org/wiki/Backpropagation) for training neural networks.

In this guide, you will explore ways to compute gradients with TensorFlow, especially in eager execution.

Setup

```
import numpy as np
import matplotlib.pyplot as plt

import tensorflow as tf
```

Computing gradients

To differentiate automatically, TensorFlow needs to remember what operations happen in what order during the *forward* pass. Then, during the *backward pass*, TensorFlow traverses this list of operations in reverse order to compute gradients.

Gradient tapes

TensorFlow provides the `tf.GradientTape` (https://www.tensorflow.org/api_docs/python/tf/GradientTape) API for automatic differentiation; that is, computing the gradient of a computation with respect to some inputs, usually `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable)s. TensorFlow "records" relevant operations executed inside the context of a `tf.GradientTape` (https://www.tensorflow.org/api_docs/python/tf/GradientTape) onto a "tape". TensorFlow then uses that tape to compute the gradients of a "recorded" computation using reverse mode differentiation (https://en.wikipedia.org/wiki/Automatic_differentiation).

Here is a simple example:

```
x = tf.Variable(3.0)

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

Once you've recorded some operations, use **`GradientTape.gradient(target, sources)`** (https://www.tensorflow.org/api_docs/python/tf/GradientTape#gradient) to calculate the gradient of some target (often a loss) relative to some source (often the model's variables):

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

```
6.0
```

The above example uses scalars, but **`tf.GradientTape`** (https://www.tensorflow.org/api_docs/python/tf/GradientTape) works as easily on any tensor:

```
w = tf.Variable(tf.random.normal((3, 2)), name='w')
b = tf.Variable(tf.zeros(2, dtype=tf.float32), name='b')
x = [[1., 2., 3.]]

with tf.GradientTape(persistent=True) as tape:
  y = x @ w + b
  loss = tf.reduce_mean(y**2)
```

To get the gradient of `loss` with respect to both variables, you can pass both as sources to the `gradient` method. The tape is flexible about how sources are passed and will accept any nested combination of lists or dictionaries and return the gradient structured the same way (see **`tf.nest`** (https://www.tensorflow.org/api_docs/python/tf/nest)).

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

The gradient with respect to each source has the shape of the source:

```
print(w.shape)
print(dl_dw.shape)
```

```
(3, 2)
(3, 2)
```

Here is the gradient calculation again, this time passing a dictionary of variables:

```
my_vars = {
    'w': w,
    'b': b
}

grad = tape.gradient(loss, my_vars)
grad['b']
```

```
<tf.Tensor: shape=(2,), dtype=float32, numpy=array([3.4719186, 4.412185 ], dtype=float32)>
```

Gradients with respect to a model

It's common to collect `tf.Variables` into a `tf.Module` (https://www.tensorflow.org/api_docs/python/tf/Module) or one of its subclasses (`layers.Layer` (https://www.tensorflow.org/api_docs/python/tf/keras/layers/Layer), `keras.Model` (https://www.tensorflow.org/api_docs/python/tf/keras/Model)) for checkpointing (/guide/checkpoint) and exporting (/guide/saved_model).

In most cases, you will want to calculate gradients with respect to a model's trainable variables. Since all subclasses of `tf.Module` (https://www.tensorflow.org/api_docs/python/tf/Module) aggregate their variables in the `Module.trainable_variables` (https://www.tensorflow.org/api_docs/python/tf/Module#trainable_variables) property, you can calculate these gradients in a few lines of code:

```
layer = tf.keras.layers.Dense(2, activation='relu')
x = tf.constant([[1., 2., 3.]])

with tf.GradientTape() as tape:
  # Forward pass
  y = layer(x)
  loss = tf.reduce_mean(y**2)

# Calculate gradients with respect to every trainable variable
grad = tape.gradient(loss, layer.trainable_variables)
```

```
for var, g in zip(layer.trainable_variables, grad):
  print(f'{var.name}, shape: {g.shape}')
```

```
dense/kernel:0, shape: (3, 2)
dense/bias:0, shape: (2,)
```

Controlling what the tape watches

The default behavior is to record all operations after accessing a trainable `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable). The reasons for this are:

- The tape needs to know which operations to record in the forward pass to calculate the gradients in the backwards pass.
- The tape holds references to intermediate outputs, so you don't want to record unnecessary operations.
- The most common use case involves calculating the gradient of a loss with respect to all a model's trainable variables.

For example, the following fails to calculate a gradient because the `tf.Tensor` (https://www.tensorflow.org/api_docs/python/tf/Tensor) is not "watched" by default, and the `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable) is not trainable:

```
# 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:
  y = (x0**2) + (x1**2) + (x2**2)

grad = tape.gradient(y, [x0, x1, x2, x3])

for g in grad:
  print(g)
```

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

You can list the variables being watched by the tape using the `GradientTape.watched_variables` (https://www.tensorflow.org/api_docs/python/tf/GradientTape#watched_variables) method:

```
[var.name for var in tape.watched_variables()]
```

```
['x0:0']
```

`tf.GradientTape` (https://www.tensorflow.org/api_docs/python/tf/GradientTape) provides hooks that give the user control over what is or is not watched.

To record gradients with respect to a `tf.Tensor` (https://www.tensorflow.org/api_docs/python/tf/Tensor), you need to call `GradientTape.watch(x)` (https://www.tensorflow.org/api_docs/python/tf/GradientTape#watch):

```
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())
```

```
6.0
```

Conversely, to disable the default behavior of watching all `tf.Variables`, set `watch_accessed_variables=False` when creating the gradient tape. This calculation uses two variables, but only connects the gradient for one of the variables:

```
x0 = tf.Variable(0.0)
x1 = tf.Variable(10.0)

with tf.GradientTape(watch_accessed_variables=False) as tape:
  tape.watch(x1)
  y0 = tf.math.sin(x0)
  y1 = tf.nn.softplus(x1)
  y = y0 + y1
  ys = tf.reduce_sum(y)
```

Since `GradientTape.watch` (https://www.tensorflow.org/api_docs/python/tf/GradientTape#watch) was not called on `x0`, no gradient is computed with respect to it:

```
# dys/dx1 = exp(x1) / (1 + exp(x1)) = sigmoid(x1)
grad = tape.gradient(ys, {'x0': x0, 'x1': x1})

print('dy/dx0:', grad['x0'])
print('dy/dx1:', grad['x1'].numpy())
```

```
dy/dx0: None
dy/dx1: 0.9999546
```

Intermediate results

You can also request gradients of the output with respect to intermediate values computed inside the `tf.GradientTape` (https://www.tensorflow.org/api_docs/python/tf/GradientTape) context.

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

```
18.0
```

By default, the resources held by a `GradientTape` are released as soon as the `GradientTape.gradient` (https://www.tensorflow.org/api_docs/python/tf/GradientTape#gradient) method is called. To compute multiple gradients over the same computation, create a gradient tape with `persistent=True`. This allows multiple calls to the `gradient` method as resources are released when the tape object is garbage collected. For example:

```
x = tf.constant([1, 3.0])
with tf.GradientTape(persistent=True) as tape:
  tape.watch(x)
  y = x * x
  z = y * y

print(tape.gradient(z, x).numpy())  # [4.0, 108.0] (4 * x**3 at x = [1.0, 3.0])
print(tape.gradient(y, x).numpy())  # [2.0, 6.0] (2 * x at x = [1.0, 3.0])
```

```
[  4. 108.]
[2. 6.]
```

```
del tape   # Drop the reference to the tape
```

Notes on performance

- There is a tiny overhead associated with doing operations inside a gradient tape context. For most eager execution this will not be a noticeable cost, but you should still use tape context around the areas only where it is required.
- Gradient tapes use memory to store intermediate results, including inputs and outputs, for use during the backwards pass.

  For efficiency, some ops (like `ReLU`) don't need to keep their intermediate results and they are pruned during the forward pass. However, if you use `persistent=True` on your tape, *nothing is discarded* and your peak memory usage will be higher.

Gradients of non-scalar targets

A gradient is fundamentally an operation on a scalar.

```
x = tf.Variable(2.0)
with tf.GradientTape(persistent=True) as tape:
  y0 = x**2
  y1 = 1 / x

print(tape.gradient(y0, x).numpy())
print(tape.gradient(y1, x).numpy())
```

```
4.0
-0.25
```

Thus, if you ask for the gradient of multiple targets, the result for each source is:

- The gradient of the sum of the targets, or equivalently
- The sum of the gradients of each target.

```
x = tf.Variable(2.0)
with tf.GradientTape() as tape:
  y0 = x**2
  y1 = 1 / x

print(tape.gradient({'y0': y0, 'y1': y1}, x).numpy())
```

```
3.75
```

Similarly, if the target(s) are not scalar the gradient of the sum is calculated:

```
x = tf.Variable(2.)

with tf.GradientTape() as tape:
  y = x * [3., 4.]

print(tape.gradient(y, x).numpy())
```

```
7.0
```

This makes it simple to take the gradient of the sum of a collection of losses, or the gradient of the sum of an element-wise loss calculation.

If you need a separate gradient for each item, refer to Jacobians (/guide/advanced_autodiff#jacobians).

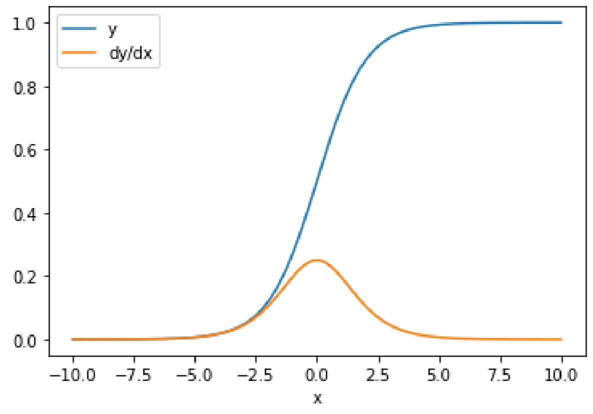
In some cases you can skip the Jacobian. For an element-wise calculation, the gradient of the sum gives the derivative of each element with respect to its input-element, since each element is independent:

```
x = tf.linspace(-10.0, 10.0, 200+1)

with tf.GradientTape() as tape:
  tape.watch(x)
  y = tf.nn.sigmoid(x)

dy_dx = tape.gradient(y, x)
```

```
plt.plot(x, y, label='y')
plt.plot(x, dy_dx, label='dy/dx')
plt.legend()
_ = plt.xlabel('x')
```



Control flow

Because a gradient tape records operations as they are executed, Python control flow is naturally handled (for example, `if` and `while` statements).

Here a different variable is used on each branch of an `if`. The gradient only connects to the variable that was used:

```
x = tf.constant(1.0)

v0 = tf.Variable(2.0)
v1 = tf.Variable(2.0)

with tf.GradientTape(persistent=True) as tape:
  tape.watch(x)
  if x > 0.0:
    result = v0
  else:
    result = v1**2

dv0, dv1 = tape.gradient(result, [v0, v1])

print(dv0)
print(dv1)
```

```
tf.Tensor(1.0, shape=(), dtype=float32)
None
```

Just remember that the control statements themselves are not differentiable, so they are invisible to gradient-based optimizers.

Depending on the value of `x` in the above example, the tape either records `result = v0` or `result = v1**2`. The gradient with respect to `x` is always `None`.

```
dx = tape.gradient(result, x)

print(dx)
```

```
None
```

Cases where `gradient` returns `None`

When a target is not connected to a source, `gradient` will return `None`.

```
x = tf.Variable(2.)
y = tf.Variable(3.)

with tf.GradientTape() as tape:
  z = y * y
print(tape.gradient(z, x))
```

```
None
```

Here `z` is obviously not connected to `x`, but there are several less-obvious ways that a gradient can be disconnected.

1. Replaced a variable with a tensor

In the section on "controlling what the tape watches" (#watches) you saw that the tape will automatically watch a `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable) but not a `tf.Tensor` (https://www.tensorflow.org/api_docs/python/tf/Tensor).

One common error is to inadvertently replace a `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable) with a `tf.Tensor` (https://www.tensorflow.org/api_docs/python/tf/Tensor), instead of using `Variable.assign` (https://www.tensorflow.org/api_docs/python/tf/Variable#assign) to update the `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable). Here is an example:

```
x = tf.Variable(2.0)

for epoch in range(2):
  with tf.GradientTape() as tape:
    y = x+1

  print(type(x).__name__, ":", tape.gradient(y, x))
  x = x + 1   # This should be `x.assign_add(1)`
```

```
ResourceVariable : tf.Tensor(1.0, shape=(), dtype=float32)
EagerTensor : None
```

2. Did calculations outside of TensorFlow

The tape can't record the gradient path if the calculation exits TensorFlow. For example:

```
x = tf.Variable([[1.0, 2.0],
                 [3.0, 4.0]], dtype=tf.float32)

with tf.GradientTape() as tape:
  x2 = x**2

  # This step is calculated with NumPy
  y = np.mean(x2, axis=0)

  # Like most ops, reduce_mean will cast the NumPy array to a constant tensor
  # using `tf.convert_to_tensor`.
  y = tf.reduce_mean(y, axis=0)

print(tape.gradient(y, x))
```

```
None
```

3. Took gradients through an integer or string

Integers and strings are not differentiable. If a calculation path uses these data types there will be no gradient.

Nobody expects strings to be differentiable, but it's easy to accidentally create an `int` constant or variable if you don't specify the `dtype`.

```
x = tf.constant(10)

with tf.GradientTape() as g:
  g.watch(x)
  y = x * x

print(g.gradient(y, x))
```

```
WARNING:tensorflow:The dtype of the watched tensor must be floating (e.g. tf.float32), got tf.int
WARNING:tensorflow:The dtype of the target tensor must be floating (e.g. tf.float32) when calling
WARNING:tensorflow:The dtype of the source tensor must be floating (e.g. tf.float32) when calling
None
```

TensorFlow doesn't automatically cast between types, so, in practice, you'll often get a type error instead of a missing gradient.

4. Took gradients through a stateful object

State stops gradients. When you read from a stateful object, the tape can only observe the current state, not the history that lead to it.

A `tf.Tensor` (https://www.tensorflow.org/api_docs/python/tf/Tensor) is immutable. You can't change a tensor once it's created. It has a *value*, but no *state*. All the operations discussed so far are also stateless: the output of a `tf.matmul` (https://www.tensorflow.org/api_docs/python/tf/linalg/matmul) only depends on its inputs.

A `tf.Variable` (https://www.tensorflow.org/api_docs/python/tf/Variable) has internal state—its value. When you use the variable, the state is read. It's normal to calculate a gradient with respect to a variable, but the variable's state blocks gradient calculations from going farther back. For example:

```
x0 = tf.Variable(3.0)
x1 = tf.Variable(0.0)

with tf.GradientTape() as tape:
  # Update x1 = x1 + x0.
  x1.assign_add(x0)
  # The tape starts recording from x1.
  y = x1**2   # y = (x1 + x0)**2

# This doesn't work.
print(tape.gradient(y, x0))   #dy/dx0 = 2*(x1 + x0)
```

```
None
```

Similarly, `tf.data.Dataset` (https://www.tensorflow.org/api_docs/python/tf/data/Dataset) iterators and `tf.queue` (https://www.tensorflow.org/api_docs/python/tf/queue)s are stateful, and will stop all gradients on tensors that pass through them.

No gradient registered

Some `tf.Operation` (https://www.tensorflow.org/api_docs/python/tf/Operation)s are **registered as being non-differentiable** and will return `None`. Others have **no gradient registered**.

The `tf.raw_ops` (https://www.tensorflow.org/api_docs/python/tf/raw_ops) page shows which low-level ops have gradients registered.

If you attempt to take a gradient through a float op that has no gradient registered the tape will throw an error instead of silently returning `None`. This way you know something has gone wrong.

For example, the `tf.image.adjust_contrast` (https://www.tensorflow.org/api_docs/python/tf/image/adjust_contrast) function wraps `raw_ops.AdjustContrastv2` (https://www.tensorflow.org/api_docs/python/tf/raw_ops/AdjustContrastv2), which could have a gradient but the gradient is not implemented:

```
image = tf.Variable([[[0.5, 0.0, 0.0]]])
delta = tf.Variable(0.1)

with tf.GradientTape() as tape:
  new_image = tf.image.adjust_contrast(image, delta)

try:
  print(tape.gradient(new_image, [image, delta]))
  assert False   # This should not happen.
except LookupError as e:
  print(f'{type(e).__name__}: {e}')
```

```
LookupError: gradient registry has no entry for: AdjustContrastv2
```

If you need to differentiate through this op, you'll either need to implement the gradient and register it (using `tf.RegisterGradient` (https://www.tensorflow.org/api_docs/python/tf/RegisterGradient)) or re-implement the function using other ops.

Zeros instead of None

In some cases it would be convenient to get 0 instead of `None` for unconnected gradients. You can decide what to return when you have unconnected gradients using the `unconnected_gradients` argument:

```
x = tf.Variable([2., 2.])
y = tf.Variable(3.)

with tf.GradientTape() as tape:
  z = y**2
print(tape.gradient(z, x, unconnected_gradients=tf.UnconnectedGradients.ZERO))
```

```
tf.Tensor([0. 0.], shape=(2,), dtype=float32)
```