EE-559 – Deep learning 4.2. Autograd

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Conceptually, the forward pass is a standard tensor computation, and the DAG of tensor operations is required only to compute derivatives.

When executing tensor operations, PyTorch can automatically construct on-the-fly the graph of operations to compute the gradient of any quantity with respect to any tensor involved.

This "autograd" mechanism (Paszke et al., 2017) has two main benefits:

- Simpler syntax: one just need to write the forward pass as a standard sequence of Python operations,
- greater flexibility: since the graph is not static, the forward pass can be dynamically modulated.

A Tensor has a Boolean field requires_grad, set to False by default, which states if PyTorch should build the graph of operations so that gradients with respect to it can be computed.

The result of a tensorial operation has this flag to True if any of its operand has it to True.

```
>>> x = torch.tensor([ 1., 2. ])
>>> y = torch.tensor([ 4., 5. ])
>>> z = torch.tensor([ 7., 3. ])
>>> x.requires_grad
False
>>> (x + y).requires_grad
False
>>> z.requires_grad = True
>>> (x + z).requires_grad
True
```

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Only floating point type tensors can have their gradient computed.

```
>>> x = torch.tensor([1., 10.])
>>> x.requires_grad = True
>>> x = torch.tensor([1, 10])
>>> x.requires_grad = True
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
RuntimeError: only Tensors of floating point dtype can require gradients
```

The method requires_grad_(value = True) set requires_grad to value, which is True by default.

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torch.autograd.grad(outputs, inputs) computes and returns the gradient of outputs with respect to inputs.

```
>>> t = torch.tensor([1., 2., 4.]).requires_grad_()
>>> u = torch.tensor([10., 20.]).requires_grad_()
>>> a = t.pow(2).sum() + u.log().sum()
>>> torch.autograd.grad(a, (t, u))
(tensor([2., 4., 8.]), tensor([0.1000, 0.0500]))
```

inputs can be a single tensor, but the result is still a [one element] tuple.

If outputs is a tuple, the result is the sum of the gradients of its elements.

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The function Tensor.backward() accumulates gradients in the grad fields of tensors which are not results of operations, the "leaves" in the autograd graph.

```
>>> x = torch.tensor([ -3., 2., 5. ]).requires_grad_()
>>> u = x.pow(3).sum()
>>> x.grad
>>> u.backward()
>>> x.grad
tensor([27., 12., 75.])
```

This function is an alternative to torch.autograd.grad(...) and standard for training models.

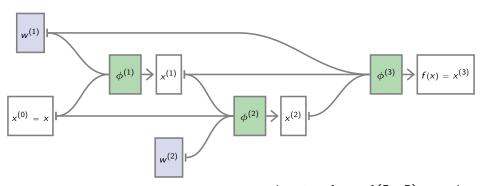


Tensor.backward() accumulates the gradients in the different Tensors, so one may have to set them to zero before calling it.

This accumulating behavior is desirable in particular to compute the gradient of a loss summed over several "mini-batches," or the gradient of a sum of losses.

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So we can run a forward/backward pass on



$$\phi^{(1)}\left(x^{(0)}; w^{(1)}\right) = w^{(1)}x^{(0)}$$

$$\phi^{(2)}\left(x^{(0)}, x^{(1)}; w^{(2)}\right) = x^{(0)} + w^{(2)}x^{(1)}$$

$$\phi^{(3)}\left(x^{(1)}, x^{(2)}; w^{(1)}\right) = w^{(1)}\left(x^{(1)} + x^{(2)}\right)$$

q.backward()

The autograd machinery

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The autograd graph is encoded through the fields grad_fn of Tensors, and the fields next_functions of Functions.

```
>>> x = torch.tensor([ 1.0, -2.0, 3.0, -4.0 ]).requires_grad_()
>>> a = x.abs()
>>> s = a.sum()
>>> s
tensor(10., grad_fn=<SumBackward0>)
>>> s.grad_fn.next_functions
((<AbsBackward object at 0x7ffb2b1462b0>, 0),)
>>> s.grad_fn.next_functions[0][0].next_functions
((<AccumulateGrad object at 0x7ffb2b146278>, 0),)
```

We will come back to this later to write our own Functions.

We can visualize the full graph built during a computation.

```
x = torch.tensor([1., 2., 2.]).requires_grad_()
q = x.norm()
AccumulateGrad

x = torch.tensor([1., 2., 2.]).requires_grad_()
q = x.norm()
```

q []

This graph was generated with

 ${\tt https://fleuret.org/git/agtree2dot} \\ and {\tt Graphviz}.$

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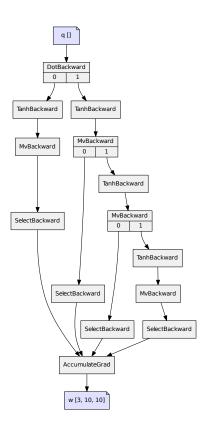
```
loss []
                                                                        MeanBackward1
                                                                        PowBackward0
                                                                        ThSubBackward
w1 = torch.rand(20, 10).requires_grad_()
b1 = torch.rand(20).requires_grad_()
                                                                         TanhBackward
w2 = torch.rand(5, 20).requires_grad_()
b2 = torch.rand(5).requires_grad_()
x = torch.rand(10)
h = torch.tanh(w1 @ x + b1)
                                                                              AccumulateGrad
y = torch.tanh(w2 @ h + b2)
                                                          AccumulateGrad
                                                                      TanhBackward
                                                                                b2 [5]
target = torch.rand(5)
                                                                     ThAddBackward
loss = (y - target).pow(2).mean()
                                                            w2 [5, 20]
                                                                 MvBackward
                                                                          AccumulateGrad
                                                                AccumulateGrad
                                                                             b1 [20]
                                                                 w1 [20, 10]
```

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```
w = torch.rand(3, 10, 10).requires_grad_()

def blah(k, x):
    for i in range(k):
        x = torch.tanh(w[i] @ x)
    return x

u = blah(1, torch.rand(10))
v = blah(3, torch.rand(10))
q = u.dot(v)
```



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Although they are related, **the autograd graph is not the network's structure**, but the graph of operations to compute the gradient. It can be data-dependent and miss or replicate sub-parts of the network.

The torch.no_grad() context switches off the autograd machinery, and can be used for operations such as parameter updates.

```
w = torch.empty(10, 784).normal_(0, 1e-3).requires_grad_()
b = torch.empty(10).normal_(0, 1e-3).requires_grad_()

for k in range(10001):
    y_hat = x @ w.t() + b
    loss = (y_hat - y).pow(2).mean()

    w.grad, b.grad = None, None
    loss.backward()

    with torch.no_grad():
        w -= eta * w.grad
        b -= eta * b.grad
```

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The detach() method creates a tensor which shares the data, but does not require gradient computation, and is not connected to the current graph.

This method should be used when the gradient should not be propagated beyond a variable, or to update leaf tensors.

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```
a = torch.tensor( 0.5).requires_grad_()
b = torch.tensor(-0.5).requires_grad_()

for k in range(100):
    1 = (a - 1)**2 + (b + 1)**2 + (a - b)**2
    ga, gb = torch.autograd.grad(1, (a, b))
    with torch.no_grad():
        a -= eta * ga
        b -= eta * gb

print('%.06f' % a.item(), '%.06f' % b.item())

prints

0.333333 -0.3333333
```

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```
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```

```
a = torch.tensor( 0.5).requires_grad_()
b = torch.tensor(-0.5).requires_grad_()

for k in range(100):
    1 = (a - 1)**2 + (b + 1)**2 + (a.detach() - b)**2
    ga, gb = torch.autograd.grad(1, (a, b))
    with torch.no_grad():
        a -= eta * ga
        b -= eta * gb

print('%.06f' % a.item(), '%.06f' % b.item())
```

1.000000 -0.000000

Autograd can also track the computation of the gradient itself, to allows **higher-order derivatives**. This is specified with create_graph = True:

```
>>> x = torch.tensor([ 1., 2., 3. ]).requires_grad_()
>>> phi = x.pow(2).sum()
>>> g1, = torch.autograd.grad(phi, x, create_graph = True)
>>> g1
tensor([2., 4., 6.], grad_fn=<ThMulBackward>)
>>> psi = g1[0].exp() - g1[2].exp()
>>> g2, = torch.autograd.grad(psi, x)
>>> g2
tensor([ 14.7781,  0.0000, -806.8576])
```

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In-place operations may corrupt values required to compute the gradient, and this is tracked down by autograd.

```
>>> x = torch.tensor([1., 2., 3.]).requires_grad_()
>>> y = x.sin()
>>> 1 = y.sum()
>>> 1.backward()
>>> y = x.sin()
>>> y += 1
>>> 1 = y.sum()
>>> 1.backward()
>>> y = x.sin()
>>> y *= y
>>> 1 = y.sum()
>>> 1.backward()
Traceback (most recent call last):
/.../
RuntimeError: one of the variables needed for gradient computation has
been modified by an inplace operation
```

They are also prohibited on so-called "leaf" tensors, which are not the results of operations but the initial inputs to the whole computation.

References

A. Paszke, S. Gross, S. Chintala, G. Chanan, E. Yang, Z. DeVito, Z. Lin, A. Desmaison, L. Antiga, and A. Lerer. Automatic differentiation in pytorch. In *Proceedings of the NIPS Autodiff workshop*, 2017.