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 needs 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
```

⚠ 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):
/.../
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.

`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.

Notes

We have

$$a(t, u) = \sum_i t_i^2 + \sum_i \log u_i$$

and we have

$$\forall i, \quad \frac{\partial a}{\partial t_i} = 2t_i$$
$$\frac{\partial a}{\partial u_i} = \frac{1}{u_i}$$

which is what is returned by `torch.autograd.grad(a, (t, u))`.

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.

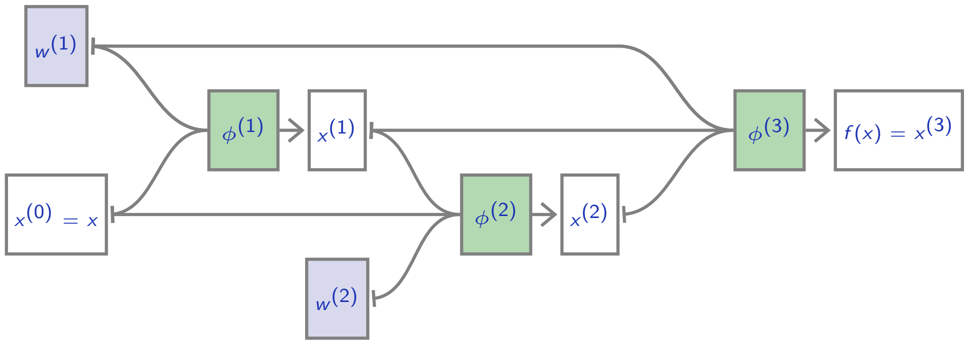
Notes

`Tensor.grad()` is useful in context of deep-learning where the main use is gradient descent, because we need to subtract the gradient of a tensor to the tensor itself.
To do so with `autograd.grad()`, we would have to associate every gradient to its tensor.

⚠ `Tensor.backward()` **accumulates** the gradients in the `grad` fields of 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.

So we can run a forward/backward pass on



$$\phi^{(1)}\left(x^{(0)}; w^{(1)}\right) = w^{(1)} x^{(0)}$$
$$\phi^{(2)}\left(x^{(0)}, x^{(1)}; w^{(2)}\right) = x^{(0)} + w^{(2)} x^{(1)}$$
$$\phi^{(3)}\left(x^{(1)}, x^{(2)}; w^{(1)}\right) = w^{(1)}\left(x^{(1)} + x^{(2)}\right)$$

```
w1 = torch.rand(5, 5).requires_grad_()
w2 = torch.rand(5, 5).requires_grad_()
x = torch.randn(5)

x0 = x
x1 = w1 @ x0
x2 = x0 + w2 @ x1
x3 = w1 @ (x1 + x2)

q = x3.norm()

q.backward()
```

Notes

The difference between Tensorflow (as we saw in lecture 4.1. “DAG networks”) and PyTorch here is that variable `q` actually contains the result of the computation.
During the tensor operations, PyTorch built all the necessary operations to compute the gradient if needed.
When calling `q.backward()`, PyTorch actually runs this built graph to fill the `grad` fields of the parameters.

The autograd machinery

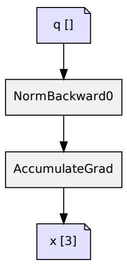
The autograd graph is encoded through the fields `grad_fn` of `Tensor`s, and the fields `next_functions` of `Function`s.

```
>>> 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 `Function`s.

We can visualize the full graph built during a computation.

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



This graph was generated with

https://fleuret.org/git/agtree2dot

and Graphviz.

Notes

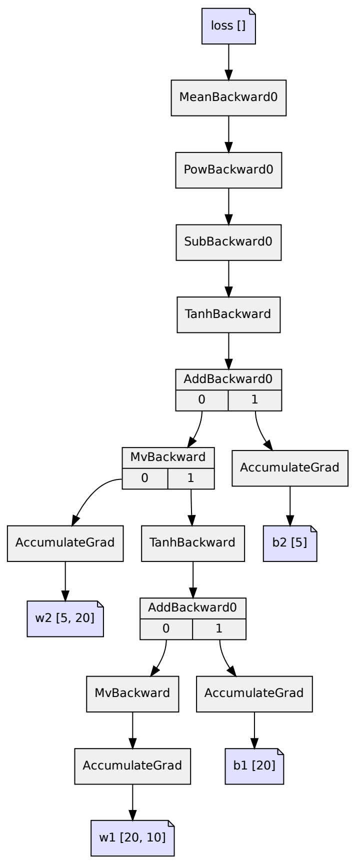
The graphs depicted here and in the coming slides show the computational graph built automatically by autograd to allow the computation of the gradient of the final value w.r.t. the initial values. `AccumulateGrad` is a particular operator that adds the values it gets if the `grad` fields. All the other blocks correspond directly to a tensor operation.

```
w1 = torch.rand(20, 10).requires_grad_()
b1 = torch.rand(20).requires_grad_()
w2 = torch.rand(5, 20).requires_grad_()
b2 = torch.rand(5).requires_grad_()

x = torch.rand(10)
h = torch.tanh(w1 @ x + b1)
y = torch.tanh(w2 @ h + b2)

targets = torch.rand(5)

loss = (y - targets).pow(2).mean()
```



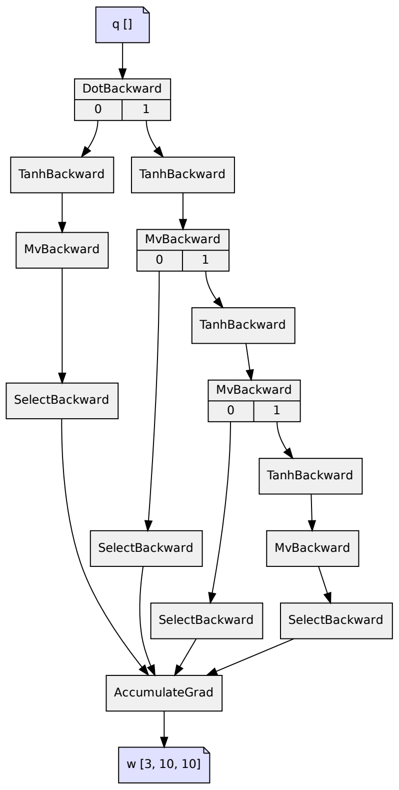
Notes

This is an implementation of a one hidden layer MLP with the tanh activation function.
Note that the block `SubBackward0` corresponds to `y - target` and gets a single output since we do no compute derivatives w.r.t. its second operand `target`.

```
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)
```



Notes

This example is more complicated and illustrates the flexibility of autograd.
Function `blah` applies a series of k matrix-vector operations and sigmoid, as specified by its operand k.
The left branch of the graph corresponds to the gradient computation of u with `k=1`, while the right part is the computation for v with `k=3`.
They all end up accumulating in the same tensor since it contains all the matrices appearing in the computation.

⚠ 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
```

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.

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

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

print(a, b)
```

prints

```
tensor(0.3333, requires_grad=True) tensor(-0.3333, requires_grad=True)
```

Notes

The loss to minimize here is:

$$\ell(a, b) = (a - 1)^2 + (b + 1)^2 + (a - b)^2$$

which leads to

$$\nabla \ell(a, b) = \begin{bmatrix} 4a - 2b - 2 \\ -2a + 4b + 2 \end{bmatrix}$$

So solving $\nabla \ell(a, b) = 0$ yields indeed $a = \frac{1}{3}$ and $b = -\frac{1}{3}$.

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

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

print(a, b)
```

prints

```
tensor(1.0000, requires_grad=True) tensor(-8.2480e-08, requires_grad=True)
```

Notes

Now, although the loss is the same, the `a.detach()` should be understood as having the same value as a but having a derivative w.r.t. a equal to zero.
Consequently the optimization finds the solution of:

$$\begin{bmatrix} 2a - 2 \\ -2a + 4b + 2 \end{bmatrix} = 0$$

By default, autograd deletes the computational graph when it is used.

```
>>> x = torch.tensor([1.]).requires_grad_()
>>> z = 1/x
>>> torch.autograd.grad(z, x)
(tensor([-1.]),)
>>> torch.autograd.grad(z * z, x)
Traceback (most recent call last):
/.../
RuntimeError: Trying to backward through the graph a second time, but
the buffers have already been freed.
```

The flag `retain_graph` indicates to keep it.

```
>>> x = torch.tensor([1.]).requires_grad_()
>>> z = 1/x
>>> torch.autograd.grad(z, x, retain_graph = True)
(tensor([-1.]),)
>>> torch.autograd.grad(z * z, x)
(tensor([-2.]),)
```

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

$$\begin{aligned}\psi(x_1, x_2) &= \log(x_1) + x_2^2 \\ \|\nabla\psi\|_2^2 &= \left(\frac{1}{x_1}\right)^2 + (2x_2)^2 \\ \nabla\|\nabla\psi\|_2^2 &= \left(-\frac{2}{x_1^3}, 8x_2\right)\end{aligned}$$

```
>>> x = torch.tensor([2., 3.]).requires_grad_()
>>> psi = x[0].log() + x[1].pow(2)
>>> g, = torch.autograd.grad(psi, x, create_graph = True)
>>> torch.autograd.grad(g.pow(2).sum(), x)
(tensor([-0.2500, 24.0000]),)
```

⚠ 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()
>>> y *= y
>>> l = y.sum()
>>> l.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.