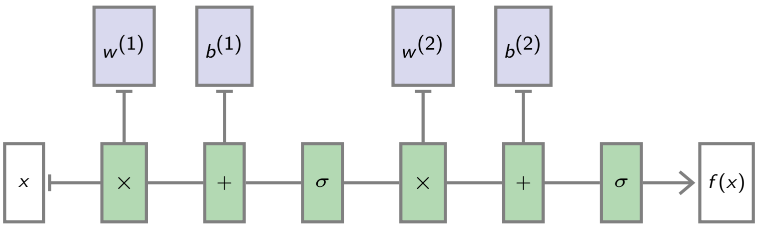
EE-559 – Deep learning

4.1. DAG networks

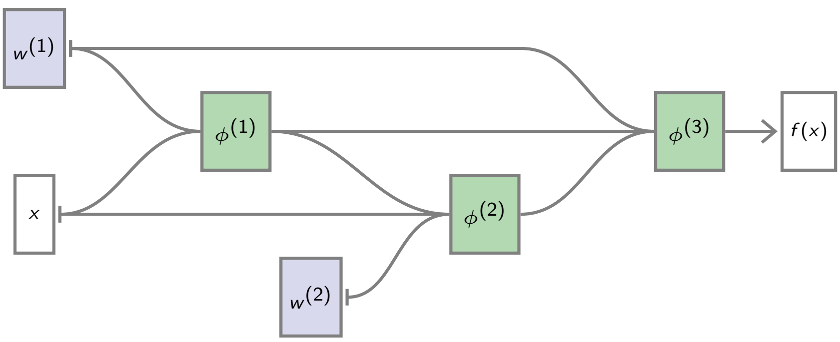
François Fleuret
`https://fleuret.org/ee559/`

Mar 10, 2020

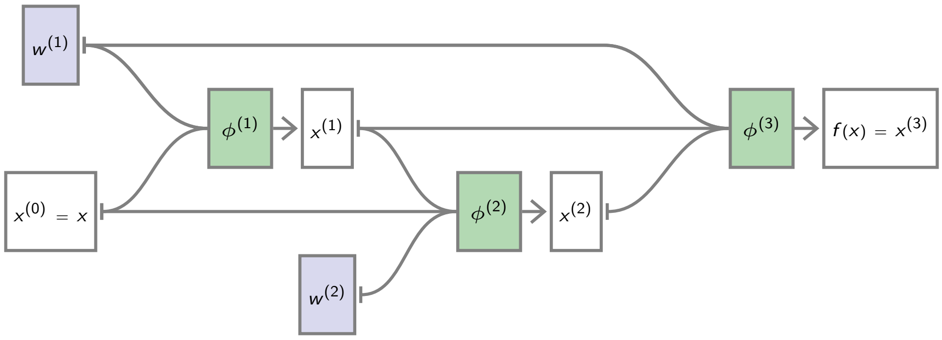
We can generalize an MLP



to an arbitrary "Directed Acyclic Graph" (DAG) of operators



Forward pass



$$
\begin{aligned}
x^{(0)} &= x \\
x^{(1)} &= \phi^{(1)}(x^{(0)}; w^{(1)}) \\
x^{(2)} &= \phi^{(2)}(x^{(0)}, x^{(1)}; w^{(2)}) \\
f(x) = x^{(3)} &= \phi^{(3)}(x^{(1)}, x^{(2)}; w^{(1)})
\end{aligned}
$$

If $(a_1, \ldots, a_Q) = \phi(b_1, \ldots, b_R)$, we use the notation

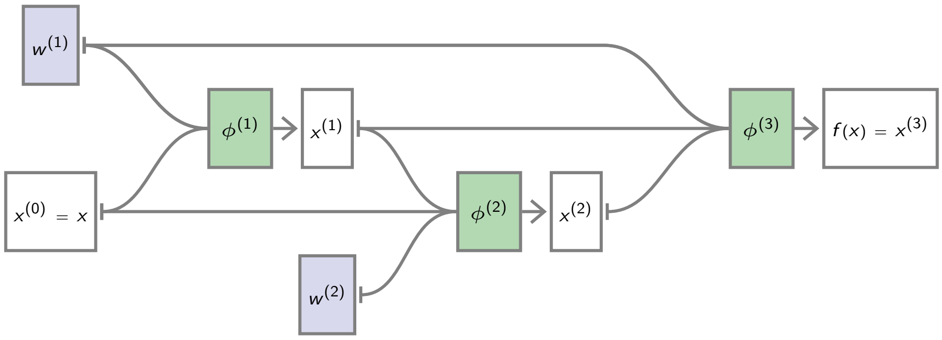
$$
\left[\frac{\partial a}{\partial b}\right] = J_\phi = \begin{pmatrix} \frac{\partial a_1}{\partial b_1} & \ldots & \frac{\partial a_1}{\partial b_R} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_Q}{\partial b_1} & \ldots & \frac{\partial a_Q}{\partial b_R} \end{pmatrix}.
$$

It does not specify at which point this is computed, but it will always be for the forward-pass activations.

Also, if $(a_1, \ldots, a_Q) = \phi(b_1, \ldots, b_R, c_1, \ldots, c_S)$, we use

$$
\left[\frac{\partial a}{\partial c}\right] = J_{\phi|c} = \begin{pmatrix} \frac{\partial a_1}{\partial c_1} & \ldots & \frac{\partial a_1}{\partial c_S} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_Q}{\partial c_1} & \ldots & \frac{\partial a_Q}{\partial c_S} \end{pmatrix}.
$$

Backward pass, derivatives w.r.t activations

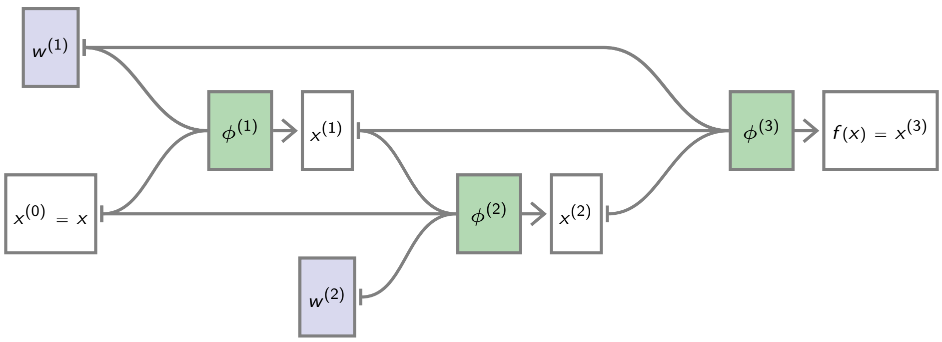


$$\left[\frac{\partial \ell}{\partial x^{(2)}}\right] = \left[\frac{\partial x^{(3)}}{\partial x^{(2)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] = J_{\phi^{(3)}|x^{(2)}}\left[\frac{\partial \ell}{\partial x^{(3)}}\right]$$

$$\left[\frac{\partial \ell}{\partial x^{(1)}}\right] = \left[\frac{\partial x^{(2)}}{\partial x^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(2)}}\right] + \left[\frac{\partial x^{(3)}}{\partial x^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] = J_{\phi^{(2)}|x^{(1)}}\left[\frac{\partial \ell}{\partial x^{(2)}}\right] + J_{\phi^{(3)}|x^{(1)}}\left[\frac{\partial \ell}{\partial x^{(3)}}\right]$$

$$\left[\frac{\partial \ell}{\partial x^{(0)}}\right] = \left[\frac{\partial x^{(1)}}{\partial x^{(0)}}\right]\left[\frac{\partial \ell}{\partial x^{(1)}}\right] + \left[\frac{\partial x^{(2)}}{\partial x^{(0)}}\right]\left[\frac{\partial \ell}{\partial x^{(2)}}\right] = J_{\phi^{(1)}|x^{(0)}}\left[\frac{\partial \ell}{\partial x^{(1)}}\right] + J_{\phi^{(2)}|x^{(0)}}\left[\frac{\partial \ell}{\partial x^{(2)}}\right]$$

Backward pass, derivatives w.r.t parameters



$$\left[\frac{\partial \ell}{\partial w^{(1)}}\right] = \left[\frac{\partial x^{(1)}}{\partial w^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(1)}}\right] + \left[\frac{\partial x^{(3)}}{\partial w^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] = J_{\phi^{(1)}|w^{(1)}}\left[\frac{\partial \ell}{\partial x^{(1)}}\right] + J_{\phi^{(3)}|w^{(1)}}\left[\frac{\partial \ell}{\partial x^{(3)}}\right]$$

$$\left[\frac{\partial \ell}{\partial w^{(2)}}\right] = \left[\frac{\partial x^{(2)}}{\partial w^{(2)}}\right]\left[\frac{\partial \ell}{\partial x^{(2)}}\right] = J_{\phi^{(2)}|w^{(2)}}\left[\frac{\partial \ell}{\partial x^{(2)}}\right]$$

So if we have a library of "tensor operators", and implementations of

$$
\begin{aligned}
(x_1, \dots, x_d, w) &\mapsto \phi(x_1, \dots, x_d; w) \\
\forall c,\ (x_1, \dots, x_d, w) &\mapsto J_{\phi|x_c}(x_1, \dots, x_d; w) \\
(x_1, \dots, x_d, w) &\mapsto J_{\phi|w}(x_1, \dots, x_d; w),
\end{aligned}
$$

we can build an arbitrary directed acyclic graph with these operators at the nodes, compute the response of the resulting mapping, and compute its gradient with back-prop.

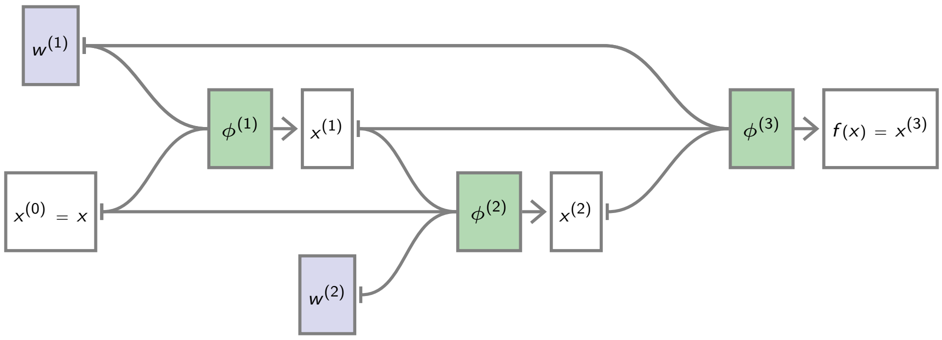
Writing from scratch a large neural network is complex and error-prone.

Multiple frameworks provide libraries of tensor operators and mechanisms to combine them into DAGs and automatically differentiate them.

	Language(s)	**License**	**Main backer**
PyTorch	**Python**	BSD	Facebook
Caffe2	C++, Python	Apache	Facebook
TensorFlow	Python, C++	Apache	Google
JAX	Python	Apache	Google
MXNet	Python, C++, R, Scala	Apache	Amazon
CNTK	Python, C++	MIT	Microsoft
Torch	Lua	BSD	Facebook
Theano	Python	BSD	U. of Montreal
Caffe	C++	BSD 2 clauses	U. of CA, Berkeley

One approach is to define the nodes and edges of such a DAG statically (Torch, TensorFlow, Caffe, Theano, etc.)

In TensorFlow, to run a forward/backward pass on



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

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

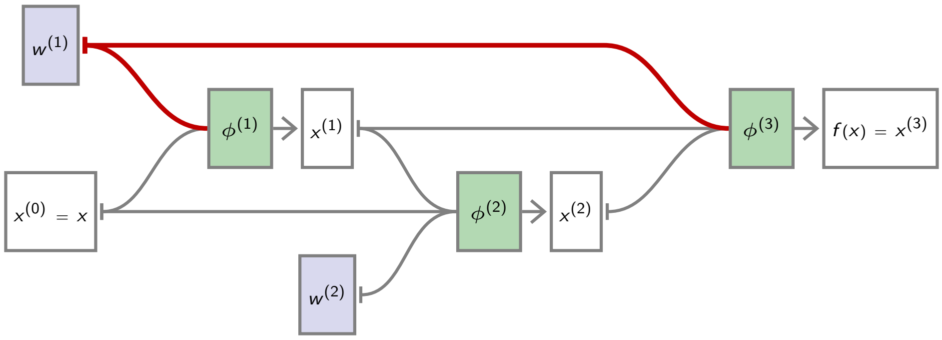
$$\phi^{(3)}\left(x^{(1)}, x^{(2)}; w^{(1)}\right) = w^{(1)}\left(x^{(1)} + x^{(2)}\right)$$

```
w1 = tf.Variable(tf.random_normal([5, 5]))
w2 = tf.Variable(tf.random_normal([5, 5]))
x = tf.Variable(tf.random_normal([5, 1]))
x0 = x
x1 = tf.matmul(w1, x0)
x2 = x0 + tf.matmul(w2, x1)
x3 = tf.matmul(w1, x1 + x2)
q = tf.norm(x3)

gw1, gw2 = tf.gradients(q, [w1, w2])

with tf.Session() as sess:
    sess.run(tf.global_variables_initializer())
    _gw1, _gw2 = sess.run([gw1, gw2])
```


Weight sharing

In our generalized DAG formulation, we have in particular implicitly allowed the same parameters to modulate different parts of the processing.

For instance $w^{(1)}$ in our example parametrizes both $\phi^{(1)}$ and $\phi^{(3)}$.



This is called **weight sharing**.

Weight sharing allows in particular to build **siamese networks** where a full sub-network is replicated several times.