Deep learning

4.1. DAG networks

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We can generalize an MLP
We can generalize an MLP

\[ w^{(1)} \times x + b^{(1)} \sigma \times w^{(2)} + b^{(2)} \sigma f(x) \]

to an arbitrary “Directed Acyclic Graph” (DAG) of operators
Forward pass

\[ f(x) = x^{(3)} \]

\[ x^{(0)} = x \]

\[ w^{(1)} \]

\[ \phi^{(1)} \rightarrow x^{(1)} \]

\[ w^{(2)} \]

\[ \phi^{(2)} \rightarrow x^{(2)} \]

\[ \phi^{(3)} \rightarrow f(x) = x^{(3)} \]
Forward pass

\[ f(x) = x(3) \]

\[ x(0) = x \]
\begin{align*}
  x^{(0)} &= x \\
  x^{(1)} &= \phi^{(1)}(x^{(0)}; w^{(1)})
\end{align*}
Forward pass

\[x^{(0)} = x\]
\[x^{(1)} = \phi^{(1)}(x^{(0)}; w^{(1)})\]
\[x^{(2)} = \phi^{(2)}(x^{(0)}, x^{(1)}; w^{(2)})\]
Forward pass

\[
x^{(0)} = x \\
x^{(1)} = \phi^{(1)}(x^{(0)}; w^{(1)}) \\
x^{(2)} = \phi^{(2)}(x^{(0)}, x^{(1)}; w^{(2)}) \\
f(x) = x^{(3)} = \phi^{(3)}(x^{(1)}, x^{(2)}; w^{(1)})
\]
If \((a_1, \ldots, a_Q) = \phi(b_1, \ldots, b_R)\), we use the notation
\[
\left[ \begin{array}{c}
\frac{\partial a}{\partial b} \\
\frac{\partial a}{\partial b_1} \quad \ldots \quad \frac{\partial a}{\partial b_R}
\end{array} \right] = J_{\phi} = 
\begin{pmatrix}
\frac{\partial a_1}{\partial b_1} & \ldots & \frac{\partial a_1}{\partial b_R} \\
\vdots & \ddots & \vdots \\
\frac{\partial a_Q}{\partial b_1} & \ldots & \frac{\partial a_Q}{\partial b_R}
\end{pmatrix}.
\]

It does not specify at which point this is computed, but it will always be for the forward-pass activations.
If \((a_1, \ldots, a_Q) = \varphi(b_1, \ldots, b_R)\), we use the notation
\[
\left[ \frac{\partial a}{\partial b} \right] = J_\varphi = \begin{pmatrix}
\frac{\partial a_1}{\partial b_1} & \cdots & \frac{\partial a_1}{\partial b_R} \\
\vdots & \ddots & \vdots \\
\frac{\partial a_Q}{\partial b_1} & \cdots & \frac{\partial a_Q}{\partial b_R}
\end{pmatrix}.
\]

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

Also, if \((a_1, \ldots, a_Q) = \varphi(b_1, \ldots, b_R, c_1, \ldots, c_S)\), we use
\[
\left[ \frac{\partial a}{\partial c} \right] = J_{\varphi|c} = \begin{pmatrix}
\frac{\partial a_1}{\partial c_1} & \cdots & \frac{\partial a_1}{\partial c_S} \\
\vdots & \ddots & \vdots \\
\frac{\partial a_Q}{\partial c_1} & \cdots & \frac{\partial a_Q}{\partial c_S}
\end{pmatrix}.
\]
Backward pass, derivatives w.r.t activations

\[
\begin{align*}
\phi(1) &= x(0) = x \\
\phi(2) &= x(1) \\
\phi(3) &= x(2) \\
f(x) &= x(3)
\end{align*}
\]
Backward pass, derivatives w.r.t activations

\[
\begin{align*}
\frac{\partial l}{\partial x(2)} &= \phi(3) \left[ \frac{\partial l}{\partial x(3)} \right] \\
&= J_{\phi(3)} | x(2) \left[ \frac{\partial l}{\partial x(3)} \right]
\end{align*}
\]
Backward pass, derivatives w.r.t activations

\[
\begin{align*}
\frac{\partial \ell}{\partial x(0)} &= \phi(3) \frac{\partial \ell}{\partial x(3)} \\
\frac{\partial \ell}{\partial x(1)} &= \phi(2) \frac{\partial \ell}{\partial x(2)} + \phi(3) \frac{\partial \ell}{\partial x(3)} \\
\frac{\partial \ell}{\partial x(2)} &= \phi(1) \frac{\partial \ell}{\partial x(1)} + \phi(2) \frac{\partial \ell}{\partial x(2)} + \phi(3) \frac{\partial \ell}{\partial x(3)}
\end{align*}
\]
Backward pass, derivatives w.r.t activations

\[
\begin{align*}
\frac{\partial \ell}{\partial x^{(0)}} &= \frac{\partial x^{(1)}}{\partial x^{(1)}} \frac{\partial \ell}{\partial x^{(1)}} + \frac{\partial x^{(2)}}{\partial x^{(0)}} \frac{\partial \ell}{\partial x^{(2)}} = J_{\phi^{(1)}} |_{x^{(0)}} \frac{\partial \ell}{\partial x^{(0)}} + J_{\phi^{(2)}} |_{x^{(0)}} \frac{\partial \ell}{\partial x^{(2)}} \\
\frac{\partial \ell}{\partial x^{(1)}} &= \frac{\partial x^{(2)}}{\partial x^{(1)}} \frac{\partial \ell}{\partial x^{(2)}} + \frac{\partial x^{(3)}}{\partial x^{(1)}} \frac{\partial \ell}{\partial x^{(3)}} = J_{\phi^{(2)}} |_{x^{(1)}} \frac{\partial \ell}{\partial x^{(2)}} + J_{\phi^{(3)}} |_{x^{(1)}} \frac{\partial \ell}{\partial x^{(3)}} \\
\frac{\partial \ell}{\partial x^{(2)}} &= \frac{\partial x^{(3)}}{\partial x^{(2)}} \frac{\partial \ell}{\partial x^{(3)}} = J_{\phi^{(3)}} |_{x^{(2)}} \frac{\partial \ell}{\partial x^{(3)}} 
\end{align*}
\]
Backward pass, derivatives w.r.t parameters

\[ x^{(0)} = x \]

\[ x^{(1)} = \phi^{(1)}(x) \]

\[ x^{(2)} = \phi^{(2)}(x) \]

\[ x^{(3)} = \phi^{(3)}(x) \]

\[ f(x) = x^{(3)} \]

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

\[ \frac{\partial l}{\partial w^{(2)}} = \left( \frac{\partial x^{(2)}}{\partial w^{(2)}} \right) \left( \frac{\partial l}{\partial x^{(2)}} \right) = J_{\phi^{(2)}} \mid_{w^{(2)}} \left( \frac{\partial l}{\partial x^{(2)}} \right) \]
Backward pass, derivatives w.r.t parameters

\[
\begin{bmatrix}
\frac{\partial \ell}{\partial w^{(1)}} \\
\frac{\partial \ell}{\partial w^{(2)}}
\end{bmatrix} =
\begin{bmatrix}
\frac{\partial x^{(1)}}{\partial w^{(1)}} \\
\frac{\partial x^{(3)}}{\partial w^{(1)}}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial \ell}{\partial x^{(1)}} \\
\frac{\partial \ell}{\partial x^{(3)}}
\end{bmatrix} +
\begin{bmatrix}
\frac{\partial x^{(1)}}{\partial w^{(2)}} \\
\frac{\partial x^{(3)}}{\partial w^{(2)}}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial \ell}{\partial x^{(1)}} \\
\frac{\partial \ell}{\partial x^{(3)}}
\end{bmatrix} = J_{\phi^{(1)}}|_{w^{(1)}} \begin{bmatrix}
\frac{\partial \ell}{\partial x^{(1)}} \\
\frac{\partial \ell}{\partial x^{(3)}}
\end{bmatrix} + J_{\phi^{(3)}}|_{w^{(1)}} \begin{bmatrix}
\frac{\partial \ell}{\partial x^{(1)}} \\
\frac{\partial \ell}{\partial x^{(3)}}
\end{bmatrix}
\]
Backward pass, derivatives w.r.t parameters

\[
\begin{align*}
\frac{\partial \ell}{\partial w^{(1)}} &= \left[ \frac{\partial x^{(1)}}{\partial w^{(1)}} \right] \left[ \frac{\partial \ell}{\partial x^{(1)}} \right] + \left[ \frac{\partial x^{(3)}}{\partial w^{(1)}} \right] \left[ \frac{\partial \ell}{\partial x^{(3)}} \right] = J_{\phi^{(1)}} |_{w^{(1)}} \left[ \frac{\partial \ell}{\partial x^{(1)}} \right] + J_{\phi^{(3)}} |_{w^{(1)}} \left[ \frac{\partial \ell}{\partial x^{(3)}} \right] \\
\frac{\partial \ell}{\partial w^{(2)}} &= \left[ \frac{\partial x^{(2)}}{\partial w^{(2)}} \right] \left[ \frac{\partial \ell}{\partial x^{(2)}} \right] = J_{\phi^{(2)}} |_{w^{(2)}} \left[ \frac{\partial \ell}{\partial x^{(2)}} \right]
\end{align*}
\]
So if we have a library of “tensor operators”, and implementations of

\[(x_1, \ldots, x_d, w) \mapsto \phi(x_1, \ldots, x_d; w)\]

\[\forall c, \ (x_1, \ldots, x_d, w) \mapsto J_{\phi|_{x_c}}(x_1, \ldots, x_d; w)\]

\[(x_1, \ldots, x_d, w) \mapsto J_{\phi|_{w}}(x_1, \ldots, x_d; w),\]
So if we have a library of “tensor operators”, and implementations of

\[(x_1, \ldots, x_d, w) \mapsto \phi(x_1, \ldots, x_d; w)\]

\[\forall c, (x_1, \ldots, x_d, w) \mapsto J_{\phi|_{x_c}}(x_1, \ldots, x_d; w)\]

\[(x_1, \ldots, x_d, w) \mapsto J_{\phi|_w}(x_1, \ldots, x_d; w),\]

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

<table>
<thead>
<tr>
<th></th>
<th>Language(s)</th>
<th>License</th>
<th>Main backer</th>
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<td>Python</td>
<td>BSD</td>
<td>Facebook</td>
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<tr>
<td>Caffe2</td>
<td>C++, Python</td>
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<tr>
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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.

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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

\[
\begin{align*}
\phi(1) & \rightarrow x(1) \\
\phi(2) & \rightarrow x(2) \\
\phi(3) & \rightarrow f(x) = x(3)
\end{align*}
\]

\[
\begin{align*}
w^{(1)} & \rightarrow \phi^{(1)} \\
w^{(2)} & \rightarrow \phi^{(2)} \\
x^{(0)} = x & \rightarrow x^{(0)} \rightarrow \phi^{(3)} \\
\end{align*}
\]
In TensorFlow, to run a forward/backward pass on

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

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

\[ \phi^{(3)} \left( x^{(1)}, x^{(2)}; w^{(1)} \right) = w^{(1)} \left( x^{(1)} + x^{(2)} \right) \]
In TensorFlow, to run a forward/backward pass on

\[
\phi^{(1)}(x^{(0)}; w^{(1)}) = w^{(1)}x^{(0)}
\]
\[
\phi^{(2)}(x^{(0)}, x^{(1)}; w^{(2)}) = x^{(0)} + w^{(2)}x^{(1)}
\]
\[
\phi^{(3)}(x^{(1)}, x^{(2)}; w^{(1)}) = w^{(1)}(x^{(1)} + x^{(2)})
\]

\[
w_1 = \text{tf.Variable}(\text{tf.random_normal}([5, 5]))
\]
\[
w_2 = \text{tf.Variable}(\text{tf.random_normal}([5, 5]))
\]
\[
x = \text{tf.Variable}(\text{tf.random_normal}([5, 1]))
\]
\[
x_0 = x
\]
\[
x_1 = \text{tf.matmul}(w_1, x_0)
\]
\[
x_2 = x_0 + \text{tf.matmul}(w_2, x_1)
\]
\[
x_3 = \text{tf.matmul}(w_1, x_1 + x_2)
\]
\[
q = \text{tf.norm}(x_3)
\]
\[
gw_1, gw_2 = \text{tf.gradients}(q, [w_1, w_2])
\]

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.

This is called weight sharing.
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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.
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The end