Deep learning

4.1. DAG networks

François Fleuret
https://fleuret.org/dlc/
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We can generalize an MLP

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

\[ \sigma(w^{(2)}(\sigma(w^{(1)}x + b^{(1)})x + b^{(2)})) \]
We can generalize an MLP

\[ \sigma \times w(1) + b(1) \times \sigma \times w(2) + b(2) \times \sigma (x) \]

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

\[ w(1) \phi(1) + w(2) \phi(2) + \phi(3) \rightarrow f(x) \]
Forward pass

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

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

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

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

It does not specify at which point this is computed, but it will always be for the forward-pass activations.
If \((a_1, \ldots, a_Q) = \phi(b_1, \ldots, b_R)\), we use the notation
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\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
\[
\left[ \frac{\partial a}{\partial c} \right] = J_{\phi|c} = \begin{pmatrix}
\frac{\partial a_1}{\partial c_1} & \cdots & \frac{\partial a_1}{\partial c_S} \\
\vdots & \ddots & \vdots \\
\frac{\partial a_Q}{\partial c_1} & \cdots & \frac{\partial a_Q}{\partial c_S}
\end{pmatrix}.
\]
Backward pass, derivatives w.r.t activations

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

\[ w^{(1)} \]

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

\[ w^{(2)} \]

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

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

\[ \phi^{(3)} \rightarrow f(x) = x^{(3)} \]
Backward pass, derivatives w.r.t activations

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

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

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

\[ w^{(1)} \rightarrow \phi^{(1)} \rightarrow x^{(1)} \rightarrow \phi^{(3)} \rightarrow f(x) = x^{(3)} \]

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

\[ w^{(2)} \rightarrow \phi^{(2)} \rightarrow x^{(2)} \]
Backward pass, derivatives w.r.t parameters

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

\[
\begin{align*}
\frac{\partial \ell}{\partial w^{(1)}} &= \left[ \frac{\partial x^{(1)}}{\partial w^{(1)}} \right] \left[ \frac{\partial \ell}{\partial x^{(1)}} \right] + \left[ \frac{\partial x^{(3)}}{\partial w^{(1)}} \right] \left[ \frac{\partial \ell}{\partial x^{(3)}} \right] = \left. J_{\phi^{(1)}} \right| w^{(1)} \left[ \frac{\partial \ell}{\partial x^{(1)}} \right] + \left. J_{\phi^{(3)}} \right| w^{(1)} \left[ \frac{\partial \ell}{\partial x^{(3)}} \right] \\
\frac{\partial \ell}{\partial w^{(2)}} &= \left[ \frac{\partial x^{(2)}}{\partial w^{(2)}} \right] \left[ \frac{\partial \ell}{\partial x^{(2)}} \right] = \left. J_{\phi^{(2)}} \right| w^{(2)} \left[ \frac{\partial \ell}{\partial x^{(2)}} \right]
\end{align*}
\]
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.

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<tr>
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<td>C++, Python</td>
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<td>BSD 2 clauses</td>
<td>U. of CA, Berkeley</td>
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In TensorFlow, to run a forward/backward pass on

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

\[
\phi^{(1)} (x^{(0)}; w^{(1)}) = w^{(1)} x^{(0)} \\
\phi^{(2)} (x^{(0)}, x^{(1)}; w^{(2)}) = x^{(0)} + w^{(2)} x^{(1)} \\
\phi^{(3)} (x^{(1)}, x^{(2)}; w^{(1)}) = w^{(1)} (x^{(1)} + x^{(2)})
\]
In TensorFlow, to run a forward/backward pass on

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

\[w^{(1)} = \text{tf.Variable(tf.random_normal([5, 5]))}\]
\[w^{(2)} = \text{tf.Variable(tf.random_normal([5, 5]))}\]
\[x = \text{tf.Variable(tf.random_normal([5, 1]))}\]
\[x^{\langle 0 \rangle} = x\]
\[x^{\langle 1 \rangle} = \text{tf.matmul}(w^{(1)}, x^{\langle 0 \rangle})\]
\[x^{\langle 2 \rangle} = x^{\langle 0 \rangle} + \text{tf.matmul}(w^{(2)}, x^{\langle 1 \rangle})\]
\[x^{\langle 3 \rangle} = \text{tf.matmul}(w^{(1)}, x^{\langle 1 \rangle} + x^{\langle 2 \rangle})\]
\[q = \text{tf.norm}(x^{\langle 3 \rangle})\]
\[gw^{(1)}, gw^{(2)} = \text{tf.gradients}(q, [w^{(1)}, w^{(2)}])\]

with \text{tf.Session()} as sess:
    \_gw^{(1)}, \_gw^{(2)} = sess.run([gw^{(1)}, gw^{(2)}])
Weight sharing
In our generalized DAG formulation, we have in particular implicitly allowed the same parameters to modulate different parts of the processing.
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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