CS490/590 Lecture 6: Backpropagation

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Spring 2020

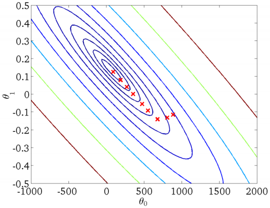
Adapted from Roger Grosse and Jimmy Ba

Overview

- We've seen that multilayer neural networks are powerful. But how can we actually learn them?
- Backpropagation is the central algorithm in this course.
  - It's is an algorithm for computing gradients.
  - Really it's an instance of reverse mode automatic differentiation, which is much more broadly applicable than just neural nets.
    - This is "just" a clever and efficient use of the Chain Rule for derivatives.
    - We'll see how to implement an automatic differentiation system next week.

Recap: Gradient Descent

- **Recall:** gradient descent moves opposite the gradient (the direction of steepest descent)



- Weight space for a multilayer neural net: one coordinate for each weight or bias of the network, in *all* the layers
- Conceptually, not any different from what we've seen so far — just higher dimensional and harder to visualize!
- We want to compute the cost gradient $\mathrm{d}\mathcal{J}/\mathrm{d}\mathbf{w}$, which is the vector of partial derivatives.
  - This is the average of $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$ over all the training examples, so in this lecture we focus on computing $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$.

Univariate Chain Rule

- We've already been using the univariate Chain Rule.
- Recall: if $f(x)$ and $x(t)$ are univariate functions, then

$$\frac{\mathrm{d}}{\mathrm{d}t}f(x(t)) = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t}.$$

Univariate Chain Rule

Recall: Univariate logistic least squares model

$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2
\end{aligned}
$$

Let's compute the loss derivatives.

Univariate Chain Rule

How you would have done it in calculus class

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2}(\sigma(wx+b)-t)^2 \\
\frac{\partial \mathcal{L}}{\partial w} &= \frac{\partial}{\partial w}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial w}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial w}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial w}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)x
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial b} &= \frac{\partial}{\partial b}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial b}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial b}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial b}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)
\end{aligned}
$$

What are the disadvantages of this approach?

Univariate Chain Rule

A more structured way to do it

Computing the loss:

$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2
\end{aligned}
$$

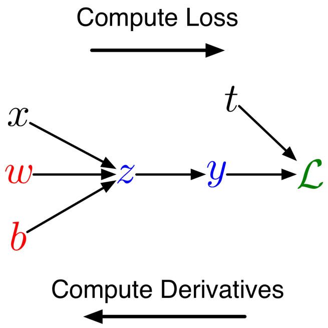
Computing the derivatives:

$$
\begin{aligned}
\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} &= y - t \\
\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\,\sigma'(z) \\
\frac{\partial\mathcal{L}}{\partial w} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}\,x \\
\frac{\partial\mathcal{L}}{\partial b} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}
\end{aligned}
$$

Remember, the goal isn't to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives.

Univariate Chain Rule

- We can diagram out the computations using a computation graph.
- The nodes represent all the inputs and computed quantities, and the edges represent which nodes are computed directly as a function of which other nodes.



Univariate Chain Rule

A slightly more convenient notation:

- Use $\overline{y}$ to denote the derivative $\mathrm{d}\mathcal{L}/\mathrm{d}y$, sometimes called the error signal.
- This emphasizes that the error signals are just values our program is computing (rather than a mathematical operation).
- This is not a standard notation, but I couldn't find another one that I liked.

Computing the loss:

$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2
\end{aligned}
$$

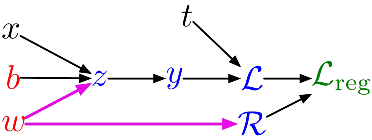
Computing the derivatives:

$$
\begin{aligned}
\overline{y} &= y - t \\
\overline{z} &= \overline{y}\, \sigma'(z) \\
\overline{w} &= \overline{z}\, x \\
\overline{b} &= \overline{z}
\end{aligned}
$$

Multivariate Chain Rule

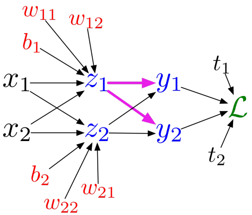
Problem: what if the computation graph has fan-out > 1?
This requires the multivariate Chain Rule!

L_2-Regularized regression



$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y-t)^2$$
$$\mathcal{R} = \frac{1}{2}w^2$$
$$\mathcal{L}_{\mathrm{reg}} = \mathcal{L} + \lambda\mathcal{R}$$

Multiclass logistic regression

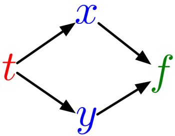


$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$
$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$
$$\mathcal{L} = -\sum_k t_k \log y_k$$

Multivariate Chain Rule

- Suppose we have a function $f(x, y)$ and functions $x(t)$ and $y(t)$. (All the variables here are scalar-valued.) Then

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t), y(t)) = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$



- Example:

$$f(x, y) = y + e^{xy}$$
$$x(t) = \cos t$$
$$y(t) = t^2$$

- Plug in to Chain Rule:

$$\begin{aligned} \frac{\mathrm{d}f}{\mathrm{d}t} &= \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t} \\ &= (ye^{xy}) \cdot (-\sin t) + (1 + xe^{xy}) \cdot 2t \end{aligned}$$

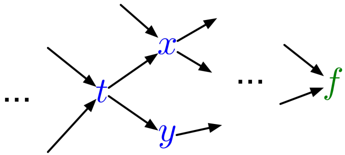
Multivariable Chain Rule

- In the context of backpropagation:

Mathematical expressions
to be evaluated

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Values already computed
by our program



- In our notation:

$$\bar{t} = \bar{x}\,\frac{\mathrm{d}x}{\mathrm{d}t} + \bar{y}\,\frac{\mathrm{d}y}{\mathrm{d}t}$$

Backpropagation

Full backpropagation algorithm:

Let $v_1, \ldots, v_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

v_N denotes the variable we're trying to compute derivatives of (e.g. loss).

forward pass

For $i = 1, \ldots, N$

Compute v_i as a function of $\mathrm{Pa}(v_i)$

backward pass

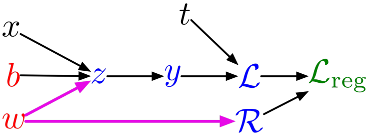
$\overline{v_N} = 1$

For $i = N - 1, \ldots, 1$

$\overline{v_i} = \sum_{j \in \mathrm{Ch}(v_i)} \overline{v_j} \frac{\partial v_j}{\partial v_i}$

Backpropagation

Example: univariate logistic least squares regression



Forward pass:

$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2 \\
\mathcal{R} &= \frac{1}{2}w^2 \\
\mathcal{L}_{\mathrm{reg}} &= \mathcal{L} + \lambda\mathcal{R}
\end{aligned}
$$

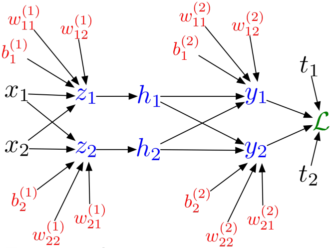
Backward pass:

$$
\begin{aligned}
\overline{\mathcal{L}_{\mathrm{reg}}} &= 1 \\
\overline{\mathcal{R}} &= \overline{\mathcal{L}_{\mathrm{reg}}}\,\frac{\mathrm{d}\mathcal{L}_{\mathrm{reg}}}{\mathrm{d}\mathcal{R}} \\
&= \overline{\mathcal{L}_{\mathrm{reg}}}\,\lambda \\
\overline{\mathcal{L}} &= \overline{\mathcal{L}_{\mathrm{reg}}}\,\frac{\mathrm{d}\mathcal{L}_{\mathrm{reg}}}{\mathrm{d}\mathcal{L}} \\
&= \overline{\mathcal{L}_{\mathrm{reg}}} \\
\overline{y} &= \overline{\mathcal{L}}\,\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} \\
&= \overline{\mathcal{L}}\,(y - t)
\end{aligned}
$$

$$
\begin{aligned}
\overline{z} &= \overline{y}\,\frac{\mathrm{d}y}{\mathrm{d}z} \\
&= \overline{y}\,\sigma'(z) \\
\overline{w} &= \overline{z}\,\frac{\partial z}{\partial w} + \overline{\mathcal{R}}\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}w} \\
&= \overline{z}\,x + \overline{\mathcal{R}}\,w \\
\overline{b} &= \overline{z}\,\frac{\partial z}{\partial b} \\
&= \overline{z}
\end{aligned}
$$

Backpropagation

Multilayer Perceptron (multiple outputs):



Forward pass:

$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

$$h_i = \sigma(z_i)$$

$$y_k = \sum_i w_{ki}^{(2)} h_i + b_k^{(2)}$$

$$\mathcal{L} = \frac{1}{2} \sum_k (y_k - t_k)^2$$

Backward pass:

$$\overline{\mathcal{L}} = 1$$

$$\overline{y_k} = \overline{\mathcal{L}}\,(y_k - t_k)$$

$$\overline{w_{ki}^{(2)}} = \overline{y_k}\, h_i$$

$$\overline{b_k^{(2)}} = \overline{y_k}$$

$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

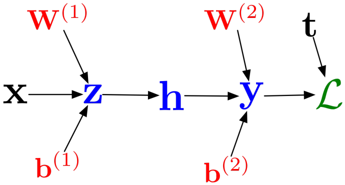
$$\overline{z_i} = \overline{h_i}\, \sigma'(z_i)$$

$$\overline{w_{ij}^{(1)}} = \overline{z_i}\, x_j$$

$$\overline{b_i^{(1)}} = \overline{z_i}$$

Vector Form

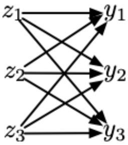
- Computation graphs showing individual units are cumbersome.
- As you might have guessed, we typically draw graphs over the vectorized variables.



- We pass messages back analogous to the ones for scalar-valued nodes.

Vector Form

- Consider this computation graph:



$$\mathbf{z} \longrightarrow \mathbf{y}$$

- Backprop rules:

$$\overline{z_j} = \sum_k \overline{y_k} \frac{\partial y_k}{\partial z_j} \qquad\qquad \overline{\mathbf{z}} = \frac{\partial \mathbf{y}}{\partial \mathbf{z}}^\top \overline{\mathbf{y}},$$

where $\partial \mathbf{y} / \partial \mathbf{z}$ is the Jacobian matrix:

$$\frac{\partial \mathbf{y}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial y_1}{\partial z_1} & \cdots & \frac{\partial y_1}{\partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial z_1} & \cdots & \frac{\partial y_m}{\partial z_n} \end{pmatrix}$$

Vector Form

Examples

- Matrix-vector product

$$\mathbf{z} = \mathbf{W}\mathbf{x} \qquad \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \mathbf{W} \qquad \overline{\mathbf{x}} = \mathbf{W}^\top \overline{\mathbf{z}}$$

- Elementwise operations

$$\mathbf{y} = \exp(\mathbf{z}) \qquad \frac{\partial \mathbf{y}}{\partial \mathbf{z}} = \begin{pmatrix} \exp(z_1) & & 0 \\ & \ddots & \\ 0 & & \exp(z_D) \end{pmatrix} \qquad \overline{\mathbf{z}} = \exp(\mathbf{z}) \circ \overline{\mathbf{y}}$$

- Note: we never explicitly construct the Jacobian. It's usually simpler and more efficient to compute the VJP directly.

Vector Form

Full backpropagation algorithm (vector form):

Let $\mathbf{v}_1, \ldots, \mathbf{v}_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

$\mathbf{v}_N$ denotes the variable we're trying to compute derivatives of (e.g. loss). It's a scalar, which we can treat as a 1-D vector.

forward pass

For $i = 1, \ldots, N$

Compute $\mathbf{v}_i$ as a function of $\mathrm{Pa}(\mathbf{v}_i)$

backward pass

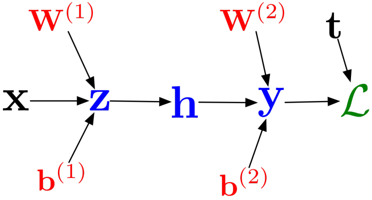
$\overline{\mathbf{v}_N} = 1$

For $i = N-1, \ldots, 1$

$$\overline{\mathbf{v}_i} = \sum_{j \in \mathrm{Ch}(\mathbf{v}_i)} \frac{\partial \mathbf{v}_j}{\partial \mathbf{v}_i}^\top \overline{\mathbf{v}_j}$$

Vector Form

MLP example in vectorized form:



Forward pass:

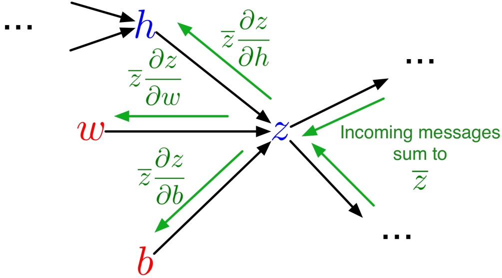
$$\begin{aligned}
\mathbf{z} &= \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)} \\
\mathbf{h} &= \sigma(\mathbf{z}) \\
\mathbf{y} &= \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)} \\
\mathcal{L} &= \frac{1}{2}\|\mathbf{t} - \mathbf{y}\|^2
\end{aligned}$$

Backward pass:

$$\begin{aligned}
\overline{\mathcal{L}} &= 1 \\
\overline{\mathbf{y}} &= \overline{\mathcal{L}}\,(\mathbf{y} - \mathbf{t}) \\
\overline{\mathbf{W}^{(2)}} &= \overline{\mathbf{y}}\mathbf{h}^\top \\
\overline{\mathbf{b}^{(2)}} &= \overline{\mathbf{y}} \\
\overline{\mathbf{h}} &= \mathbf{W}^{(2)\top}\overline{\mathbf{y}} \\
\overline{\mathbf{z}} &= \overline{\mathbf{h}} \circ \sigma'(\mathbf{z}) \\
\overline{\mathbf{W}^{(1)}} &= \overline{\mathbf{z}}\mathbf{x}^\top \\
\overline{\mathbf{b}^{(1)}} &= \overline{\mathbf{z}}
\end{aligned}$$

Backpropagation

Backprop as message passing:



- Each node receives a bunch of messages from its children, which it aggregates to get its error signal. It then passes messages to its parents.
- This provides modularity, since each node only has to know how to compute derivatives with respect to its arguments, and doesn't have to know anything about the rest of the graph.

Computational Cost

- Computational cost of forward pass: one add-multiply operation per weight

$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

- Computational cost of backward pass: two add-multiply operations per weight

$$\begin{aligned} \overline{w_{ki}^{(2)}} &= \overline{y_k}\, h_i \\ \overline{h_i} &= \sum_k \overline{y_k} w_{ki}^{(2)} \end{aligned}$$

- Rule of thumb: the backward pass is about as expensive as two forward passes.
- For a multilayer perceptron, this means the cost is linear in the number of layers, quadratic in the number of units per layer.

Closing Thoughts

- Backprop is used to train the overwhelming majority of neural nets today.
  - Even optimization algorithms much fancier than gradient descent (e.g. second-order methods) use backprop to compute the gradients.
- Despite its practical success, backprop is believed to be neurally implausible.
  - No evidence for biological signals analogous to error derivatives.
  - All the biologically plausible alternatives we know about learn much more slowly (on computers).
  - So how on earth does the brain learn?

Closing Thoughts

- By now, we've seen three different ways of looking at gradients:
    - **Geometric:** visualization of gradient in weight space
    - **Algebraic:** mechanics of computing the derivatives
    - **Implementational:** efficient implementation on the computer
- When thinking about neural nets, it's important to be able to shift between these different perspectives!