TU-Delft Deep Learning course 2018-2019

03.backprop

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Delft University of Technology

Lecturer: Jan van Gemert
Several slides credit to Roger Grosse

Learning goals

After this lecture you can:

- Understand what the goal of backpropagation is
- Explain the forward/backward pass
- Apply the calculus chain rule to compute derivatives
- Apply the backpropagation algorithm to efficiently compute derivatives
- Understand the modularity of network nodes

Book chapters: 4.3, 6.5

Training a network

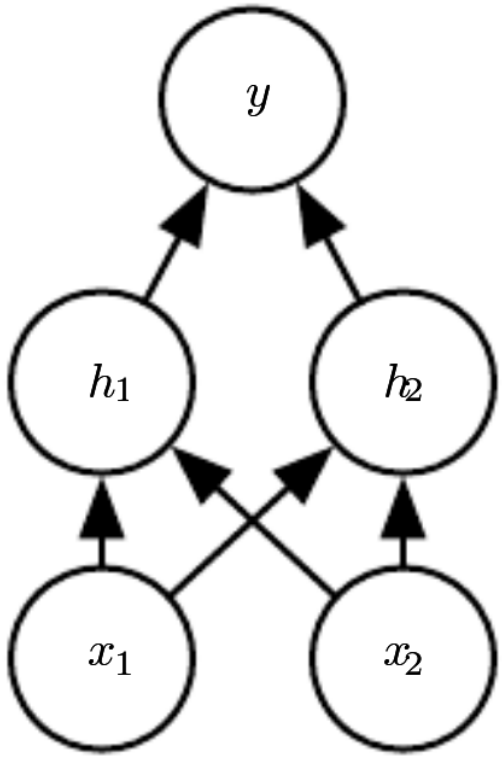
Chapter 4.3

Training set:

Data		Label
0	1	1
1	1	0
0	0	0
1	0	1

While not converged:

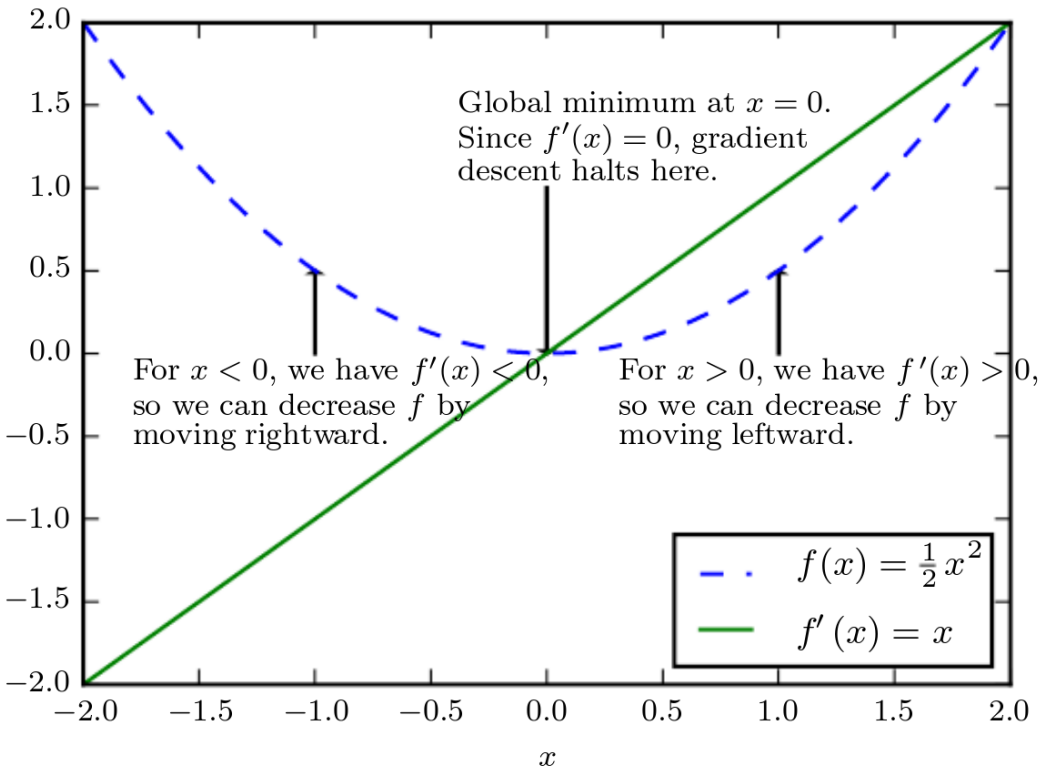
1. Present a training sample $\rightarrow$ Forward pass
2. Compare the results $\rightarrow$ Loss
3. Update the weights $\rightarrow$ Backward pass



Backward pass: Backpropagation

- Backpropagation: Efficient algorithm to compute gradients
- Used to train a huge majority of deep nets
- Engine that powers "End-to-End" optimization and representation learning
- Its "just" a clever application of the chain rule of calculus

Updating the weights: Gradient descent



1-d gradient descent

- Q: How does "1-d" change for a multi-layer network?
- A: One coordinate for each weight/bias in *all* the layers
- Compute cost gradient $\frac{d\mathcal{E}}{d\mathbf{w}}$: vector of partial derivatives
- Q: How to get cost gradient from training samples?
- A: Average $\frac{d\mathcal{L}}{d\mathbf{w}}$ for loss $\mathcal{L}$ over all training samples

Chain rule to compute derivatives

- Deep net is a function chain $f(x) = f^{(3)}(f^{(2)}(f^{(1)}(x)))$

  Q: How to compute $f(g(x))'$?
  A: $f(g(x))' = f'(g(x))g'(x)$

- Let: $y = g(x)$, and $z = f(g(x)) = f(y)$.
- Other notation:

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

- Multi-variate chain rule, let $f = (x(t), y(t))$, then

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

- Interpretation: How much does output change if the input slightly changes

Assignment: Compute loss $\mathcal{L}$ derivatives

Model: $\mathcal{L} = \frac{1}{2}\left(\sigma(\text{wx+b})\text{-t}\right)^2$, where $t =$ true label

Q: What to compute?

A: Derivative to w

$$\frac{\partial}{\partial w}\mathcal{L} = \frac{\partial}{\partial w}\left[\frac{1}{2}\left(\sigma(\text{wx+b})\text{-t}\right)^2\right]$$

$$= \left(\sigma(\text{wx+b})\text{-t}\right)\frac{\partial}{\partial w}\left(\sigma(\text{wx+b})\text{-t}\right)$$

$$= \left(\sigma(\text{wx+b})\text{-t}\right)\sigma'(\text{wx+b})\frac{\partial}{\partial w}(\text{wx+b})$$

$$= \left(\sigma(\text{wx+b})\text{-t}\right)\sigma'(\text{wx+b})x$$

A: Derivative to b

$$\frac{\partial}{\partial b}\mathcal{L} = \frac{\partial}{\partial b}\left[\frac{1}{2}\left(\sigma(\text{wx+b})\text{-t}\right)^2\right] =$$

$$\left(\sigma(\text{wx+b})\text{-t}\right)\frac{\partial}{\partial b}\left(\sigma(\text{wx+b})\text{-t}\right) =$$

$$\left(\sigma(\text{wx+b})\text{-t}\right)\sigma'(\text{wx+b})\frac{\partial}{\partial b}(\text{wx+b}) =$$

$$\left(\sigma(\text{wx+b})\text{-t}\right)\sigma'(\text{wx+b})$$

Q: What are the disadvantages of this approach?

More efficient computation of loss $\mathcal{L}$ derivatives

Model: $\mathcal{L} = \frac{1}{2}\left(\sigma(\text{wx+b})\text{-t}\right)^2$

Decompose in: $z = wx + b, \quad y = \sigma(z), \quad \mathcal{L} = \frac{1}{2}(y-t)^2$

Q: Rewrite using chain rule in terms of $\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$?

A: Derivative to w

$$\frac{d\mathcal{L}}{dw} = \frac{dL}{dy}\frac{dy}{dz}\frac{dz}{dw}$$

A: Derivative to b

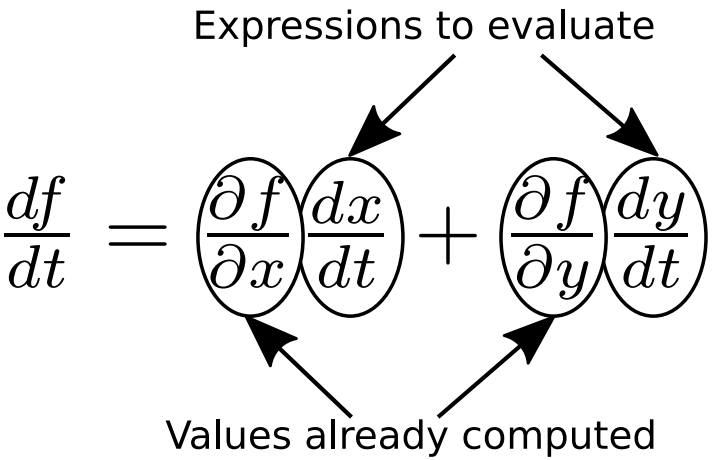
$$\frac{d\mathcal{L}}{db} = \frac{dL}{dy}\frac{dy}{dz}\frac{dz}{db}$$

Q: Nr unique terms to compute both derivatives? A: 4 (efficient re-use)

$$(1): \frac{d\mathcal{L}}{dy} = y - t, \quad (2): \frac{d\mathcal{L}}{dz} = \frac{d\mathcal{L}}{dy}\sigma'(z), \quad (3): \frac{d\mathcal{L}}{dw} = \frac{d\mathcal{L}}{dz}x, \quad (4): \frac{d\mathcal{L}}{db} = \frac{d\mathcal{L}}{dz}.$$

Q: Dependency order of computation? A: Starts backwards.

Re-using pre-computed values



Bar notation:

- Backprop is an algorithm to compute values
- Bar notation[1] for computed values: $\overline{y} = \frac{d\mathcal{E}}{dy}$
- Less cluttered and emphasizes value re-use

Example: $z = wx + b, \quad y = \sigma(z), \quad \mathcal{L} = \frac{1}{2}(y - t)^2$

Instead of:

$$(1) : \frac{d\mathcal{L}}{dy} = y - t, \quad (2) : \frac{d\mathcal{L}}{dz} = \frac{d\mathcal{L}}{dy}\sigma'(z), \quad (3) : \frac{d\mathcal{L}}{dw} = \frac{d\mathcal{L}}{dz}x, \quad (4) : \frac{d\mathcal{L}}{db} = \frac{d\mathcal{L}}{dz}.$$

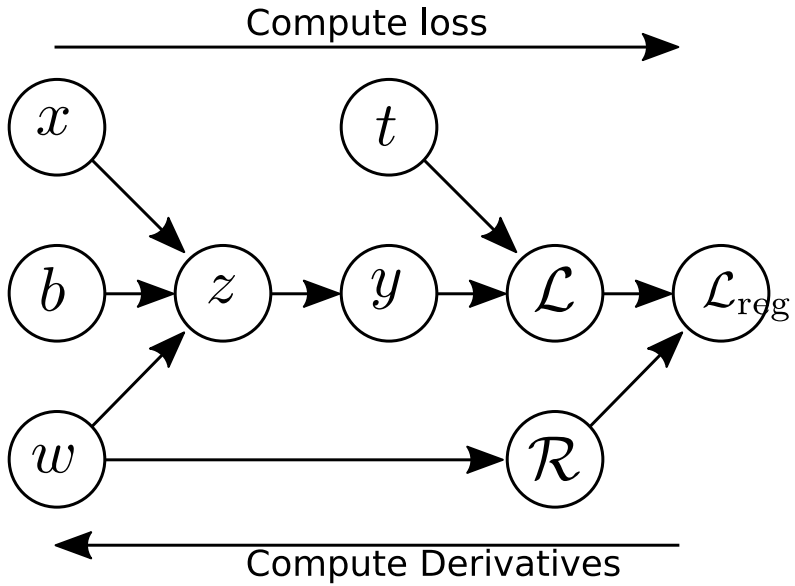
Write:

$$(1) : \overline{y} = y - t, \qquad (2) : \overline{z} = \overline{y}\sigma'(z), \qquad (3) : \overline{w} = \overline{z}x, \qquad (4) : \overline{b} = \overline{z}.$$

[1] Bar notation credits to Roger Grosse

Computational graph

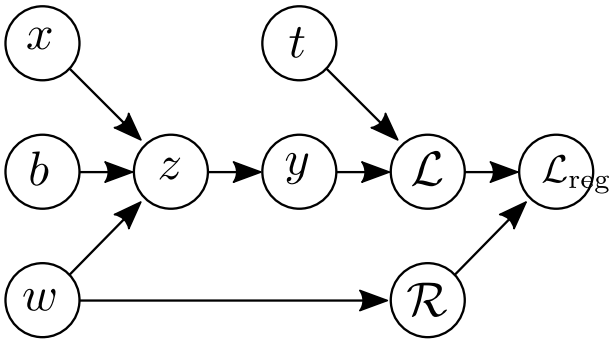
Book: Section 6.5.1



- A node is a variable: scalar, vector, matrix, tensor, other node, etc.
- An operation: simple function of 2 variables (often omitted)
- Operation have single output (possibly multiple entries)
- $x \rightarrow y$: y is computed by applying operation to x.

Backpropagation algorithm

Book: Algorithms 6.1 and 6.2



Topological ordering:
Linear ordering of vertices so for every directed edge uv, vertex u comes before v in the ordering.

Q: Topological ordering of graph?
A: $(w, b, x, z, y, t, \mathcal{L}, \mathcal{R}, \mathcal{L}_{\text{reg}})$

Backpropagation algorithm to compute gradients of node n_N:

1. Create topological ordering of graph

Forward pass $=$

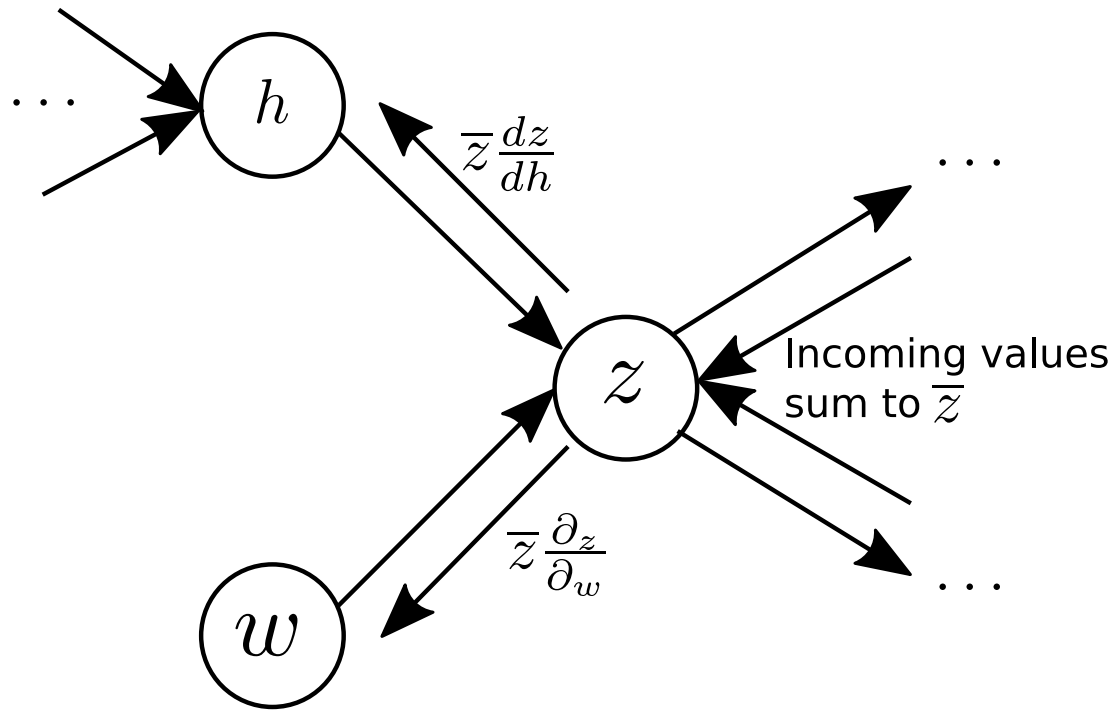
2. For $i = 1, 2, \ldots N$:
   Evaluate n_i using its function $f^{(i)}(n_i)$

Backward pass $=$

3. $\overline{n_N} = 1$ (gradient of a node wrt itself is 1; $\frac{df}{df} = 1$)
4. For $i = N - 1, \ldots 1$:
   $\overline{n_i} = \sum_{n_j \in \text{Children}(n_i)} \overline{n_j} \frac{\partial n_j}{\partial n_i}$

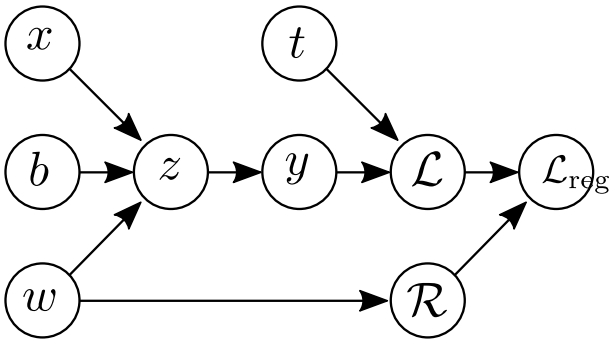
Note on step 4: node only gets gradients wrt children nodes

Backprop as message passing



- Each node aggregates the error signal from its children
- Each node passes messages to its parents
- Q: Benefit from this node-centered point of view?
- A: Modularity: Only needs to compute derivatives wrt its arguments.

Example: Univariate logistic least squares regression



Forward pass:

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

Q: Do the backward pass:

$$\overline{\mathcal{L}_{reg}} = 1$$
$$\overline{\mathcal{R}} = \overline{\mathcal{L}_{reg}}\frac{d\mathcal{L}_{reg}}{d\mathcal{R}} = \overline{\mathcal{L}_{reg}}\lambda$$
$$\overline{\mathcal{L}} = \overline{\mathcal{L}_{reg}}\frac{d\mathcal{L}_{reg}}{d\mathcal{L}} = \overline{\mathcal{L}_{reg}}$$
$$\overline{y} = \overline{\mathcal{L}}\frac{d\mathcal{L}}{dy} = \overline{\mathcal{L}}(y - t)$$
$$\overline{z} = \overline{y}\frac{dy}{dz} = \overline{y}\sigma'(z)$$
$$\overline{w} = \overline{z}\frac{\partial z}{\partial w} + \overline{\mathcal{R}}\frac{\partial \mathcal{R}}{\partial w} = \overline{z}x\overline{\mathcal{R}}w$$
$$\overline{b} = \overline{z}\frac{\partial z}{\partial b} = \overline{z}$$

Learning goals

- Understand how backpropagation powers deep learning
- Explain about the forward/backward pass
- Apply the calculus chain rule to compute derivatives
- Apply the backpropagation algorithm to efficiently compute derivatives
- Understand the modularity of network nodes