CSC 2515 Lecture 5: Neural Networks I

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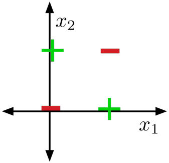
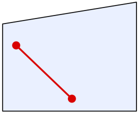
Limits of Linear Classification

- Visually, it's obvious that **XOR** is not linearly separable. But how to show this?



Limits of Linear Classification

Convex Sets



- A set $\mathcal{S}$ is convex if any line segment connecting points in $\mathcal{S}$ lies entirely within $\mathcal{S}$. Mathematically,

$$\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{S} \implies \lambda \mathbf{x}_1 + (1-\lambda)\mathbf{x}_2 \in \mathcal{S} \quad \text{for } 0 \leq \lambda \leq 1.$$

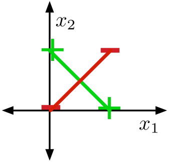
- A simple inductive argument shows that for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathcal{S}$, weighted averages, or convex combinations, lie within the set:

$$\lambda_1 \mathbf{x}_1 + \cdots + \lambda_N \mathbf{x}_N \in \mathcal{S} \quad \text{for } \lambda_i > 0, \ \lambda_1 + \cdots \lambda_N = 1.$$

Limits of Linear Classification

Showing that XOR is not linearly separable

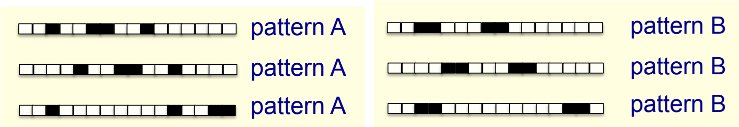
- Half-spaces are obviously convex.
- Suppose there were some feasible hypothesis. If the positive examples are in the positive half-space, then the green line segment must be as well.
- Similarly, the red line segment must line within the negative half-space.



- But the intersection can't lie in both half-spaces. Contradiction!

Limits of Linear Classification

A more troubling example



- These images represent 16-dimensional vectors. White $= 0$, black $= 1$.
- Want to distinguish patterns A and B in all possible translations (with wrap-around)
- Translation invariance is commonly desired in vision!
- Suppose there's a feasible solution. The average of all translations of A is the vector $(0.25, 0.25, \ldots, 0.25)$. Therefore, this point must be classified as A.
- Similarly, the average of all translations of B is also $(0.25, 0.25, \ldots, 0.25)$. Therefore, it must be classified as B. Contradiction!

Credit: Geoffrey Hinton

Limits of Linear Classification

- Sometimes we can overcome this limitation using feature maps, just like for linear regression. E.g., for **XOR**:

$$\boldsymbol{\psi}(\mathbf{x}) = \begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}$$

x_1	x_2	$\psi_1(\mathbf{x})$	$\psi_2(\mathbf{x})$	$\psi_3(\mathbf{x})$	t
0	0	0	0	0	0
0	1	0	1	0	1
1	0	1	0	0	1
1	1	1	1	1	0

- This is linearly separable. (Try it!)
- Not a general solution: it can be hard to pick good basis functions. Instead, we'll use neural nets to learn nonlinear hypotheses directly.

Neural Networks

Inspiration: The Brain

- Our brain has $\sim 10^{11}$ neurons, each of which communicates (is connected) to $\sim 10^4$ other neurons

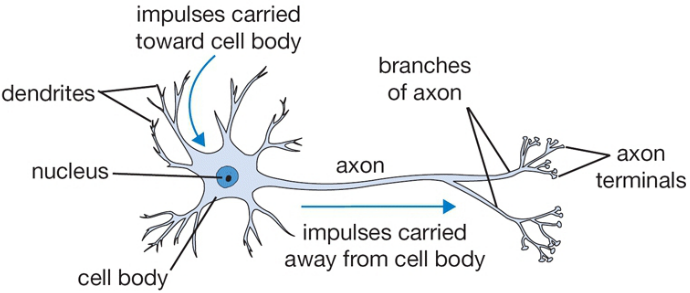
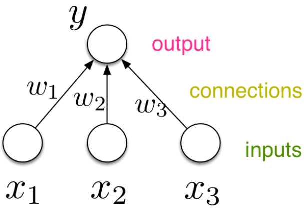

impulses carried toward cell body
dendrites
branches of axon
nucleus
axon
axon terminals
impulses carried away from cell body
cell body

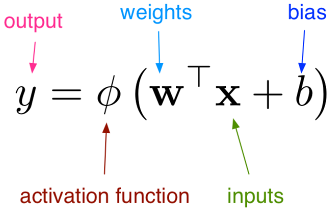
Figure: The basic computational unit of the brain: Neuron

[Pic credit: http://cs231n.github.io/neural-networks-1/]

Inspiration: The Brain

- For neural nets, we use a much simpler model neuron, or unit:





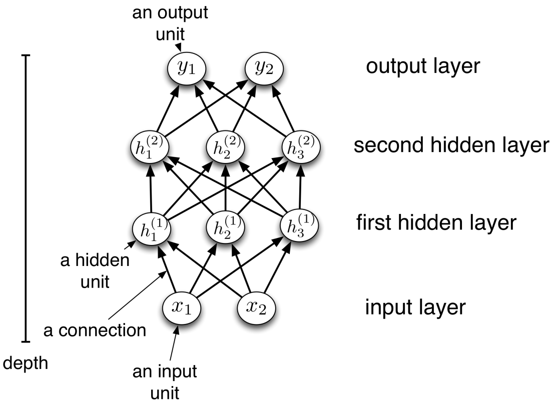
- Compare with logistic regression:

$$y = \sigma(\mathbf{w}^\top \mathbf{x} + b)$$

- By throwing together lots of these incredibly simplistic neuron-like processing units, we can do some powerful computations!

Multilayer Perceptrons

- We can connect lots of units together into a directed acyclic graph.
- This gives a feed-forward neural network. That's in contrast to recurrent neural networks, which can have cycles.
- Typically, units are grouped together into layers.



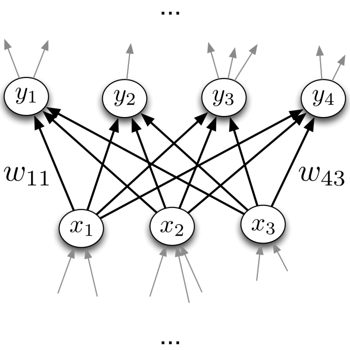
Multilayer Perceptrons

- Each layer connects N input units to M output units.
- In the simplest case, all input units are connected to all output units. We call this a fully connected layer. We'll consider other layer types later.
- Note: the inputs and outputs for a layer are distinct from the inputs and outputs to the network.

- Recall from softmax regression: this means we need an $M \times N$ weight matrix.
- The output units are a function of the input units:

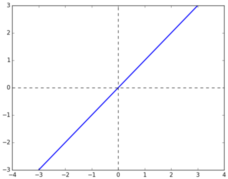
$$\mathbf{y} = f(\mathbf{x}) = \phi(\mathbf{W}\mathbf{x} + \mathbf{b})$$

- A multilayer network consisting of fully connected layers is called a multilayer perceptron. Despite the name, it has nothing to do with perceptrons!



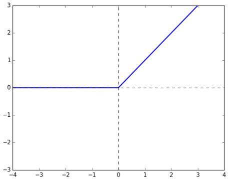
Multilayer Perceptrons

Some activation functions:



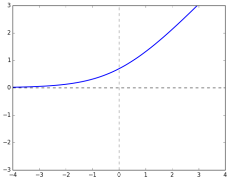
Linear

$$y = z$$



Rectified Linear Unit (ReLU)

$$y = \max(0, z)$$

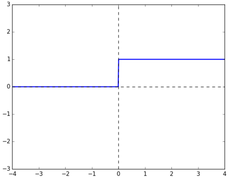


Soft ReLU

$$y = \log 1 + e^{z}$$

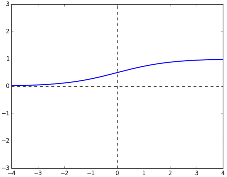
Multilayer Perceptrons

Some activation functions:



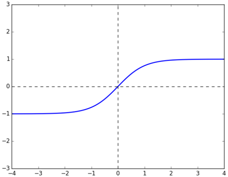
Hard Threshold

$$y = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z \leq 0 \end{cases}$$



Logistic

$$y = \frac{1}{1 + e^{-z}}$$



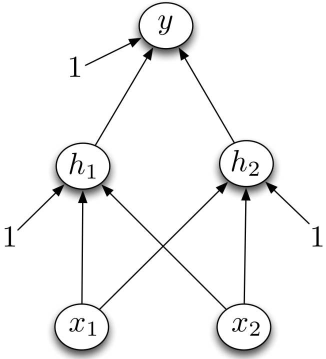
Hyperbolic Tangent (tanh)

$$y = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

Multilayer Perceptrons

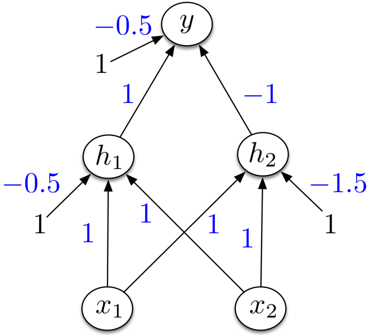
Designing a network to compute XOR:

Assume hard threshold activation function



Multilayer Perceptrons

- h_1 computes x_1 OR x_2
- h_2 computes x_1 AND x_2
- y computes h_1 AND NOT x_2



Multilayer Perceptrons

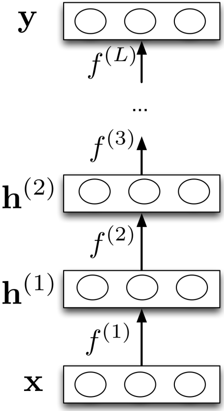
- Each layer computes a function, so the network computes a composition of functions:

$$\begin{aligned}
\mathbf{h}^{(1)} &= f^{(1)}(\mathbf{x}) \\
\mathbf{h}^{(2)} &= f^{(2)}(\mathbf{h}^{(1)}) \\
&\vdots \\
\mathbf{y} &= f^{(L)}(\mathbf{h}^{(L-1)})
\end{aligned}$$

- Or more simply:

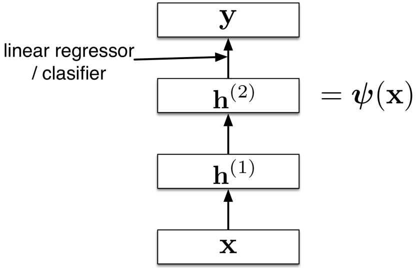
$$\mathbf{y} = f^{(L)} \circ \cdots \circ f^{(1)}(\mathbf{x}).$$

- Neural nets provide modularity: we can implement each layer's computations as a black box.



Feature Learning

- Neural nets can be viewed as a way of learning features:



$\mathbf{y}$

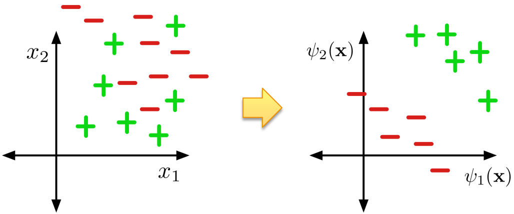
linear regressor / clasifier

$\mathbf{h}^{(2)} = \psi(\mathbf{x})$

$\mathbf{h}^{(1)}$

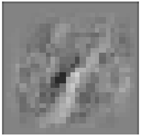
$\mathbf{x}$

- The goal:



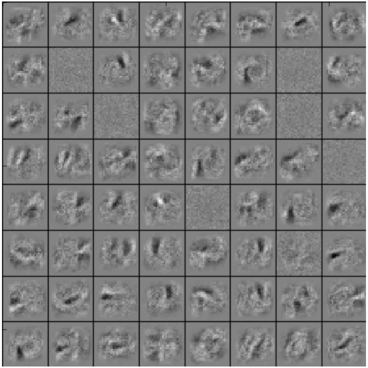
Feature Learning

- Suppose we're trying to classify images of handwritten digits. Each image is represented as a vector of $28 \times 28 = 784$ pixel values.
- Each first-layer hidden unit computes $\sigma(\mathbf{w}_i^T \mathbf{x})$. It acts as a feature detector.
- We can visualize **w** by reshaping it into an image. Here's an example that responds to a diagonal stroke.



Feature Learning

Here are some of the features learned by the first hidden layer of a handwritten digit classifier:



Expressive Power

- We've seen that there are some functions that linear classifiers can't represent. Are deep networks any better?
- Any sequence of *linear* layers can be equivalently represented with a single linear layer.

$$\mathbf{y} = \underbrace{\mathbf{W}^{(3)}\mathbf{W}^{(2)}\mathbf{W}^{(1)}}_{\triangleq \mathbf{W}'}\mathbf{x}$$

  - Deep linear networks are no more expressive than linear regression!
  - Linear layers do have their uses — stay tuned!

Expressive Power

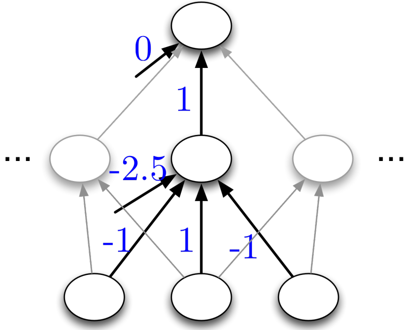
- Multilayer feed-forward neural nets with *nonlinear* activation functions are universal function approximators: they can approximate any function arbitrarily well.
- This has been shown for various activation functions (thresholds, logistic, ReLU, etc.)
    - Even though ReLU is "almost" linear, it's nonlinear enough!

Expressive Power

Universality for binary inputs and targets:

- Hard threshold hidden units, linear output
- Strategy: 2^D hidden units, each of which responds to one particular input configuration

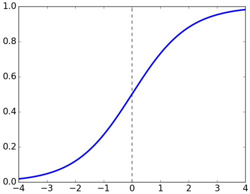
x_1	x_2	x_3	t
	$\vdots$		$\vdots$
-1	-1	1	-1
-1	1	-1	1
-1	1	1	1
	$\vdots$		$\vdots$



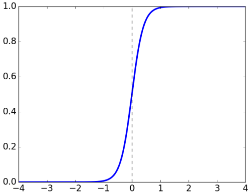
- Only requires one hidden layer, though it needs to be extremely wide!

Expressive Power

- What about the logistic activation function?
- You can approximate a hard threshold by scaling up the weights and biases:



$$y = \sigma(x)$$



$$y = \sigma(5x)$$

- This is good: logistic units are differentiable, so we can train them with gradient descent. (Stay tuned!)

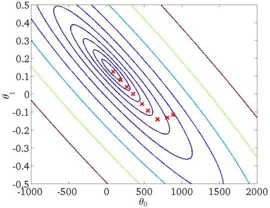
Expressive Power

- Limits of universality
  - You may need to represent an exponentially large network.
  - If you can learn any function, you'll just overfit.
  - Really, we desire a *compact* representation!
- We've derived units which compute the functions AND, OR, and NOT. Therefore, any Boolean circuit can be translated into a feed-forward neural net.
  - This suggests you might be able to learn *compact* representations of some complicated functions

Training neural networks with backpropagation

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:

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

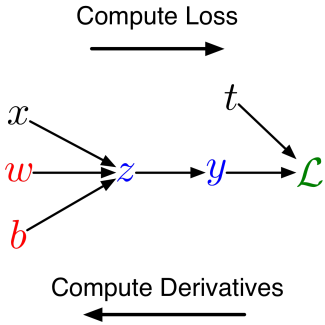
Computing the derivatives:

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

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:

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

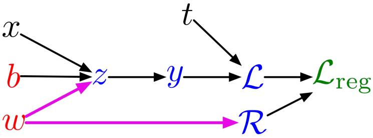
Computing the derivatives:

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

Multivariate Chain Rule

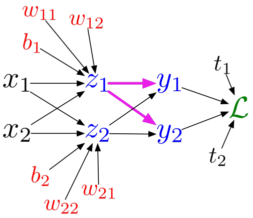
Problem: what if the computation graph has fan-out > 1?
This requires the multivariate Chain Rule!

L_2-Regularized regression



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

Softmax regression

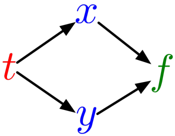


$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$
$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$
$$\mathcal{L} = -\sum_k t_k \log y_k$$

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:

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

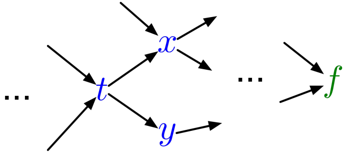
Multivariable Chain Rule

- 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:

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

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

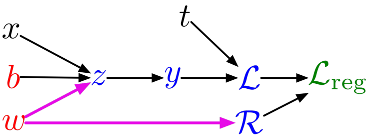
```
For $i = 1, \ldots, N$
        Compute $v_i$ as a function of $\mathrm{Pa}(v_i)$
```

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:

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

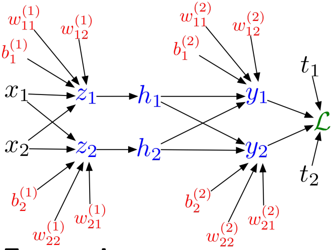
Backward pass:

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

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

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:

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

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

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

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

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

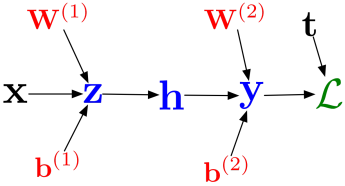
$$\overline{z_i} = \overline{h_i}\, \sigma'(z_i)$$

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

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

Vector Form

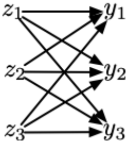
- Computation graphs showing individual units are cumbersome.
- As you might have guessed, we typically draw graphs over the vectorized variables.



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

Vector Form

- Consider this computation graph:



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

- 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

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

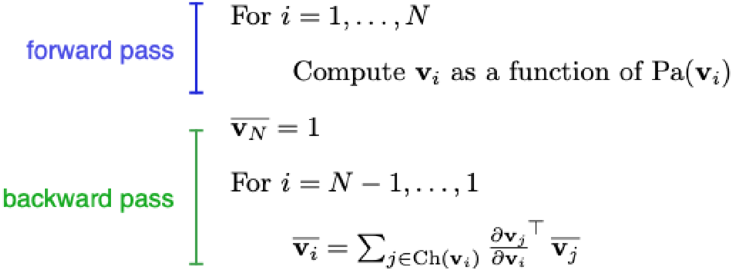
- Note: we never explicitly construct the Jacobian. It's usually simpler and more efficient to compute the vector-Jacobian product directly.

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.

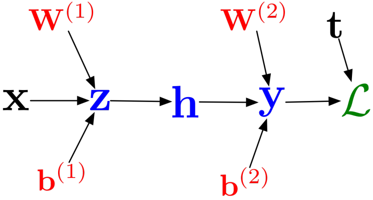


```
forward pass
    For $i = 1, \ldots, N$
        Compute $\mathbf{v}_i$ as a function of $\mathrm{Pa}(\mathbf{v}_i)$

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:

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

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.

Backpropagation

- 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?

Gradient Checking

Gradient Checking

- We've derived a lot of gradients so far. How do we know if they're correct?
- Recall the definition of the partial derivative:

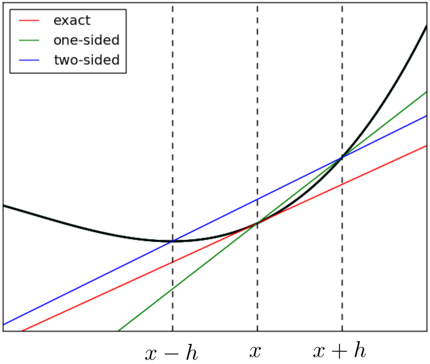
$$\frac{\partial}{\partial x_i} f(x_1, \ldots, x_N) = \lim_{h \to 0} \frac{f(x_1, \ldots, x_i + h, \ldots, x_N) - f(x_1, \ldots, x_i, \ldots, x_N)}{h}$$

- Check your derivatives numerically by plugging in a small value of h, e.g. 10^{-10}. This is known as finite differences.

Gradient Checking

- Even better: the two-sided definition

$$\frac{\partial}{\partial x_i} f(x_1, \ldots, x_N) = \lim_{h \to 0} \frac{f(x_1, \ldots, x_i + h, \ldots, x_N) - f(x_1, \ldots, x_i - h, \ldots, x_N)}{2h}$$



Gradient Checking

- Run gradient checks on small, randomly chosen inputs
- Use double precision floats (not the default for TensorFlow, PyTorch, etc.!)
- Compute the relative error:

$$\frac{|a - b|}{|a| + |b|}$$

- The relative error should be very small, e.g. 10^{-6}

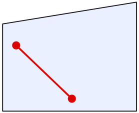
Gradient Checking

- Gradient checking is really important!
- Learning algorithms often appear to work even if the math is wrong.
- **But:**
  - They might work much better if the derivatives are correct.
  - Wrong derivatives might lead you on a wild goose chase.
- If you implement derivatives by hand, gradient checking is the single most important thing you need to do to get your algorithm to work well.

Convexity

Recap: Convex Sets

Convex Sets



- A set $\mathcal{S}$ is convex if any line segment connecting points in $\mathcal{S}$ lies entirely within $\mathcal{S}$. Mathematically,

$$\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{S} \implies \lambda \mathbf{x}_1 + (1-\lambda)\mathbf{x}_2 \in \mathcal{S} \quad \text{for } 0 \leq \lambda \leq 1.$$

- A simple inductive argument shows that for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathcal{S}$, weighted averages, or convex combinations, lie within the set:

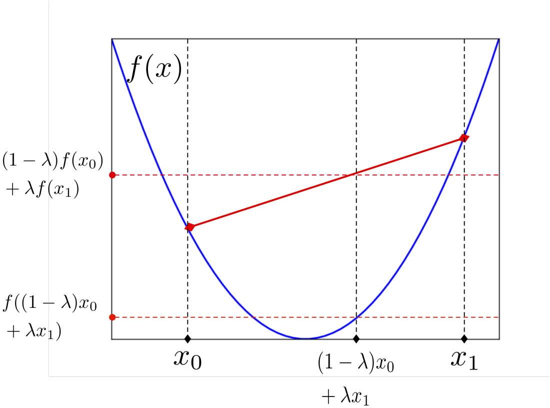
$$\lambda_1 \mathbf{x}_1 + \cdots + \lambda_N \mathbf{x}_N \in \mathcal{S} \quad \text{for } \lambda_i > 0,\ \lambda_1 + \cdots \lambda_N = 1.$$

Convex Functions

- A function f is convex if for any $\mathbf{x}_0, \mathbf{x}_1$ in the domain of f,

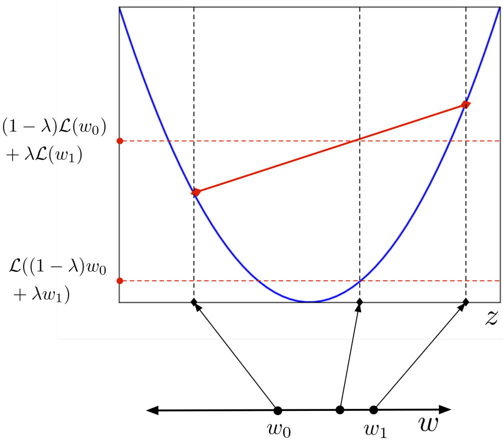
$$f((1-\lambda)\mathbf{x}_0 + \lambda\mathbf{x}_1) \leq (1-\lambda)f(\mathbf{x}_0) + \lambda f(\mathbf{x}_1)$$

- Equivalently, the set of points lying above the graph of f is convex.
- Intuitively: the function is bowl-shaped.



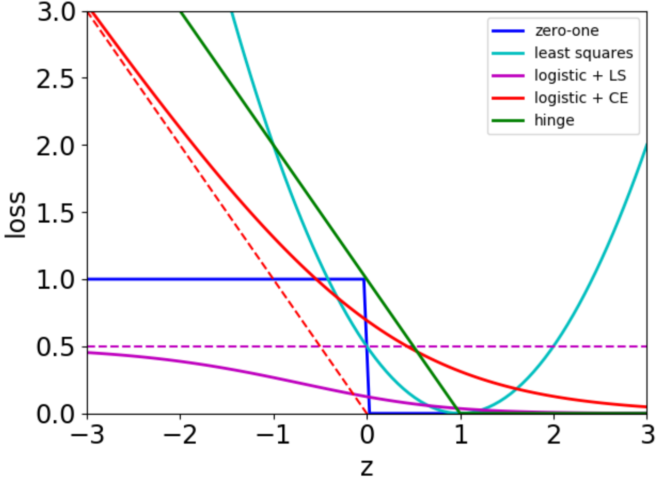
Convex Functions

- We just saw that the least-squares loss function $\frac{1}{2}(y - t)^2$ is convex as a function of y
- For a linear model, $z = \mathbf{w}^\top \mathbf{x} + b$ is a linear function of $\mathbf{w}$ and b. If the loss function is convex as a function of z, then it is convex as a function of $\mathbf{w}$ and b.


$(1-\lambda)\mathcal{L}(w_0)$
$+\lambda\mathcal{L}(w_1)$
$\mathcal{L}((1-\lambda)w_0$
$+\lambda w_1)$
z
w_0
w_1
w

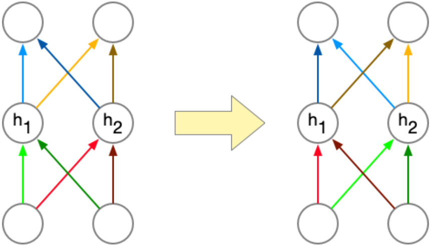
Convex Functions

Which loss functions are convex?



Local Minima

- If a function is convex, it has no spurious local minima, i.e. any local minimum is also a global minimum.
- This is very convenient for optimization since if we keep going downhill, we'll eventually reach a global minimum.
- Unfortunately, training a network with hidden units cannot be convex because of permutation symmetries.
  - I.e., we can re-order the hidden units in a way that preserves the function computed by the network.



Local Minima

- By definition, if a function $\mathcal{J}$ is convex, then for any set of points $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_N$ in its domain,

$$\mathcal{J}(\lambda_1 \boldsymbol{\theta}_1 + \cdots + \lambda_N \boldsymbol{\theta}_N) \leq \lambda_1 \mathcal{J}(\boldsymbol{\theta}_1) + \cdots + \lambda_N \mathcal{J}(\boldsymbol{\theta}_N) \quad \text{for } \lambda_i \geq 0, \sum_i \lambda_i = 1.$$

- Because of permutation symmetry, there are $K!$ permutations of the hidden units in a given layer which all compute the same function.
- Suppose we average the parameters for all $K!$ permutations. Then we get a degenerate network where all the hidden units are identical.
- If the cost function were convex, this solution would have to be better than the original one, which is ridiculous!
- Hence, training multilayer neural nets is non-convex.

Local Minima (optional, informal)

- Generally, local minima aren't something we worry much about when we train most neural nets.
- It's possible to construct arbitrarily bad local minima even for ordinary classification MLPs. It's poorly understood why these don't arise in practice.
- Intuition pump: if you have enough randomly sampled hidden units, you can approximate any function just by adjusting the output layer.
  - Then it's essentially a regression problem, which is convex.
  - Hence, local optima can probably be fixed by adding more hidden units.
  - Note: this argument hasn't been made rigorous.
- Over the past 5 years or so, CS theorists have made lots of progress proving gradient descent converges to global minima for some non-convex problems, including some specific neural net architectures.