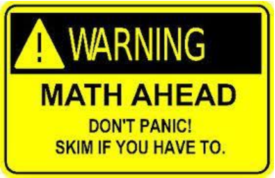
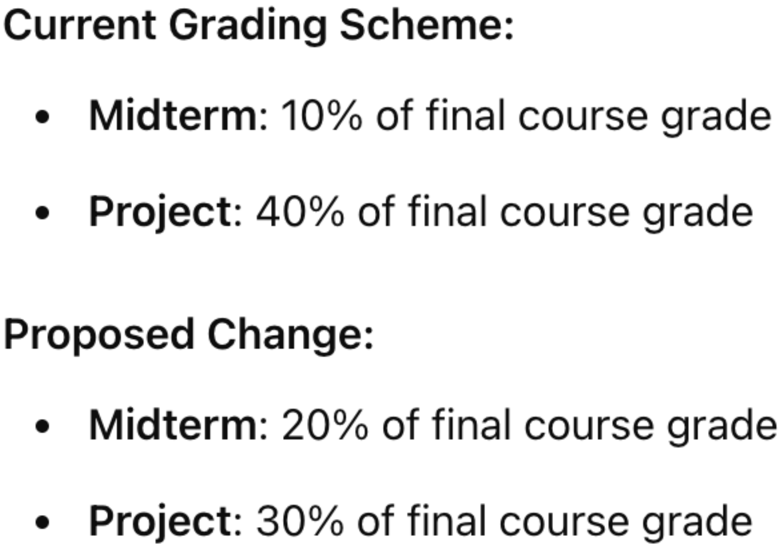


CSC413/2516 Lecture 2: Multilayer Perceptrons & Backpropagation

Bo Wang

Course information

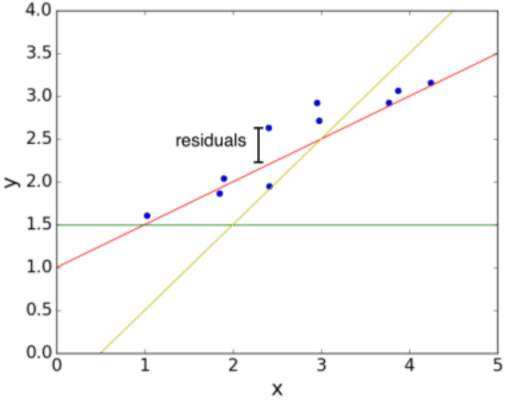


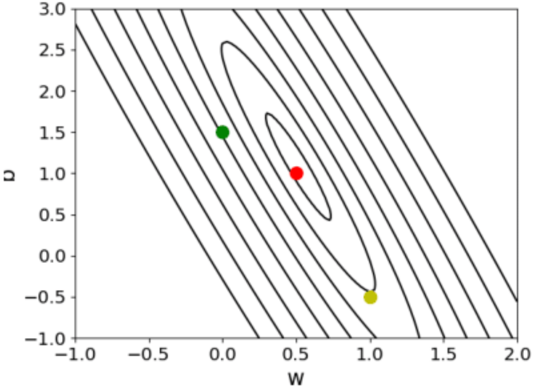
- **Current Grading Scheme:**
  - **Midterm**: 10% of final course grade
  - **Project**: 40% of final course grade

  Proposed Change:
  - **Midterm**: 20% of final course grade
  - **Project**: 30% of final course grade

- VOTING TIME!

Recap: Linear Classification and Gradient Descent

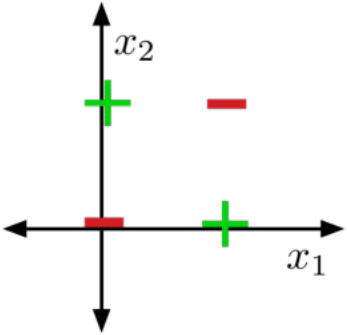




- Advantages: Easy to understand and implement; Widely-adopted;

Limits of Linear Classification

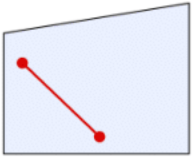
- Single neurons (linear classifiers) are very limited in expressive power.
- **XOR** is a classic example of a function that's not linearly separable.



- There's an elegant proof using convexity.

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,

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

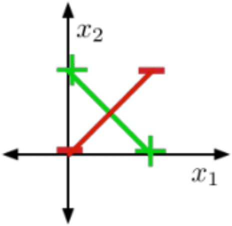
- A simple inductive argument shows that for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathcal{S}$, weighted averages, or convex combinations, lie within the set:

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

Limits of Linear Classification

Showing that XOR is not linearly separable

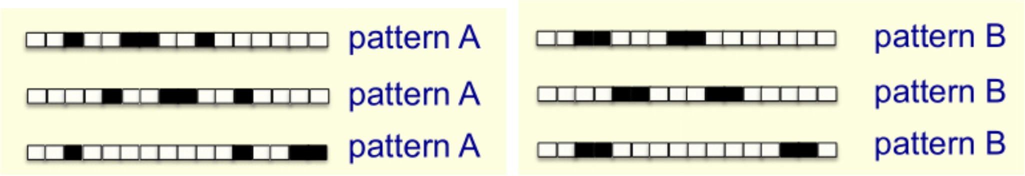
- Half-spaces are obviously convex.
- Suppose there were some feasible hypothesis. If the positive examples are in the positive half-space, then the green line segment must be as well.
- Similarly, the red line segment must line within the negative half-space.



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

Limits of Linear Classification

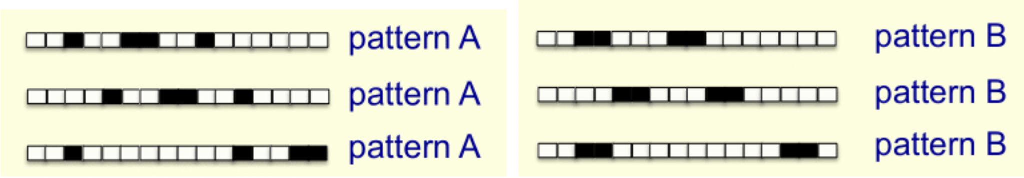
A more troubling example



- 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!

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**:

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

x_1	x_2	$\phi_1(\mathbf{x})$	$\phi_2(\mathbf{x})$	$\phi_3(\mathbf{x})$	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.

Feature maps

- We can convert linear models into nonlinear models using feature maps.

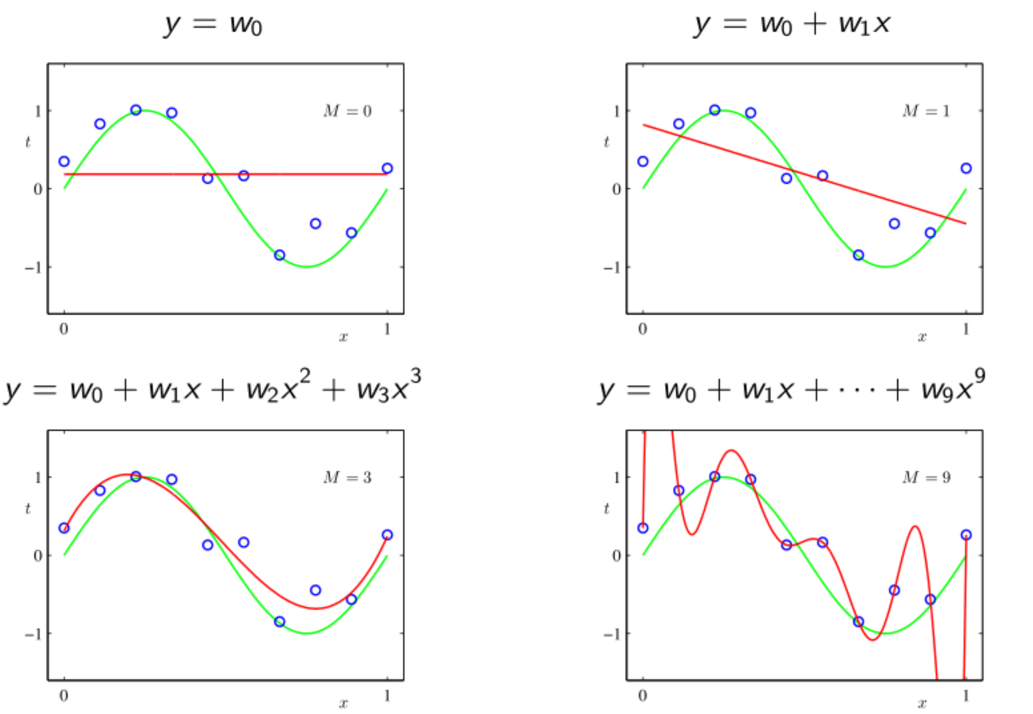
$$y = \mathrm{w}^\top \phi(\mathrm{x})$$

- E.g., if $\psi(x) = (1,\ x,\ \cdots, x^D)^\top$, then y is a polynomial in x. This model is known as polynomial regression:

$$y = w_0 + w_1 x + \cdots + w_D x^D$$

- This doesn't require changing the algorithm — just pretend $\psi(x)$ is the input vector.
- We don't need an expicit bias term, since it can be absorbed into ψ.
- Feature maps let us fit nonlinear models, but it can be hard to choose good features.
  - Before deep learning, most of the effort in building a practical machine learning system was feature engineering.

Feature maps



$$y = w_0$$

$$y = w_0 + w_1 x$$

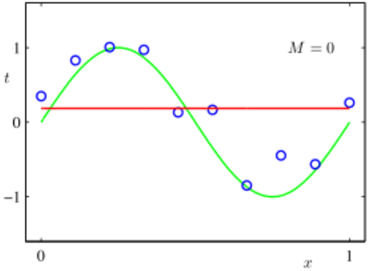
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

$$y = w_0 + w_1 x + \cdots + w_9 x^9$$

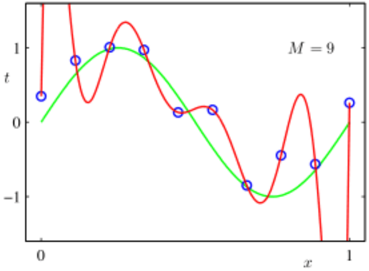
-Pattern Recognition and Machine Learning, Christopher Bishop.

Generalization

Underfitting : The model is too simple - does not fit the data.

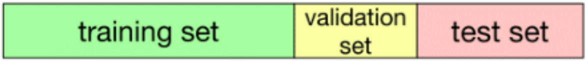


Overfitting : The model is too complex - fits perfectly, does not generalize.



Generalization

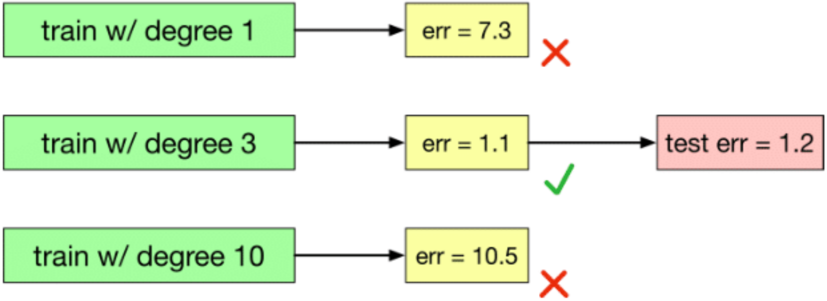
- We would like our models to generalize to data they haven't seen before
- The degree of the polynomial is an example of a hyperparameter, something we can't include in the training procedure itself
- We can tune hyperparameters using a validation set:



training set

validation set

test set

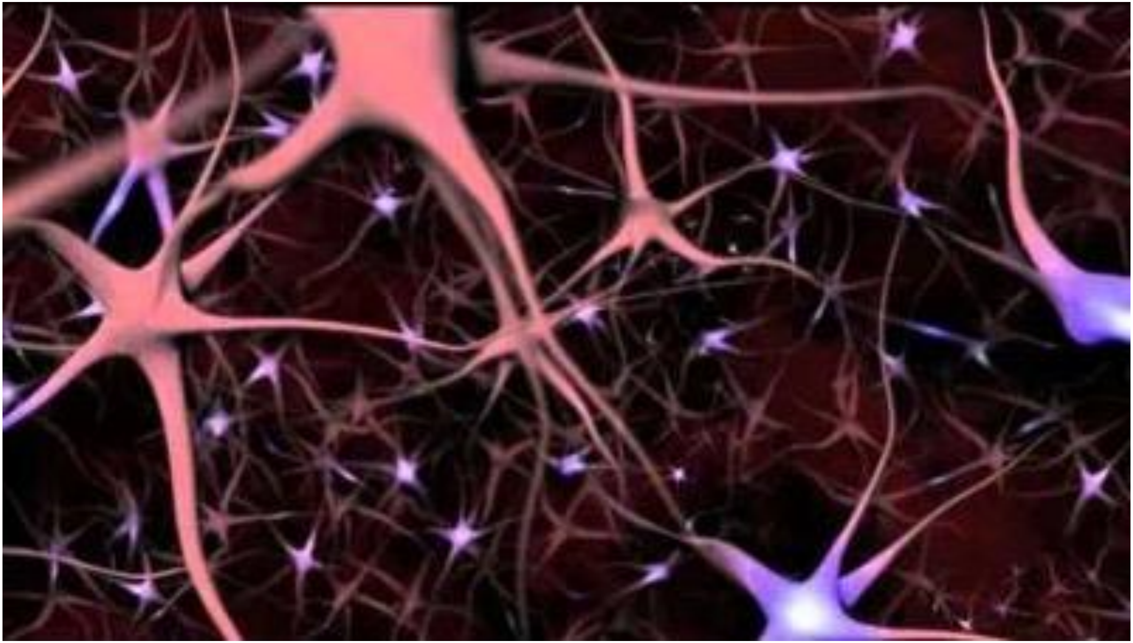


train w/ degree 1 → err = 7.3 ✗

train w/ degree 3 → err = 1.1 ✓ → test err = 1.2

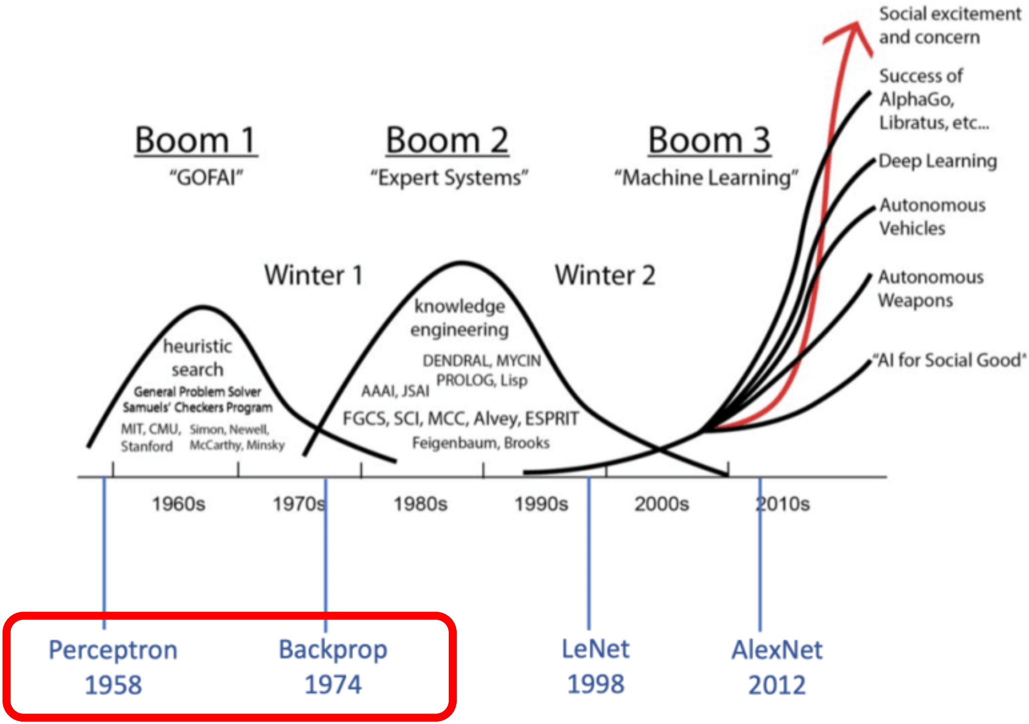
train w/ degree 10 → err = 10.5 ✗

After the break Multi-Layer Perceptrons



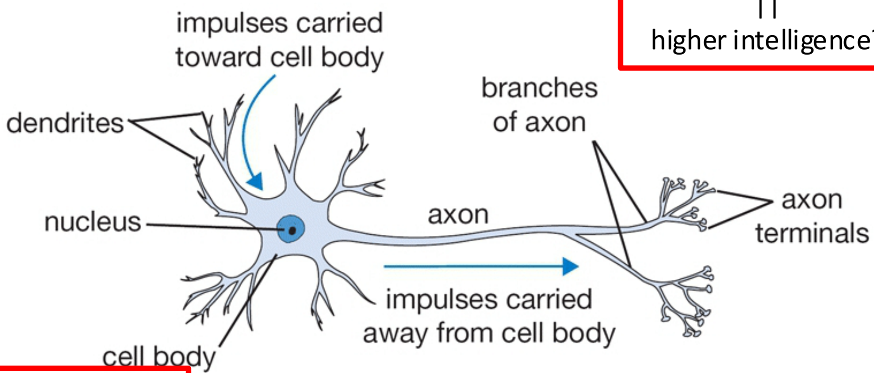
Source: https://www.youtube.com/watch?v=vyNkAuX29OU

A brief history



Multilayer Perceptrons

more neurons
||
higher intelligence?


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

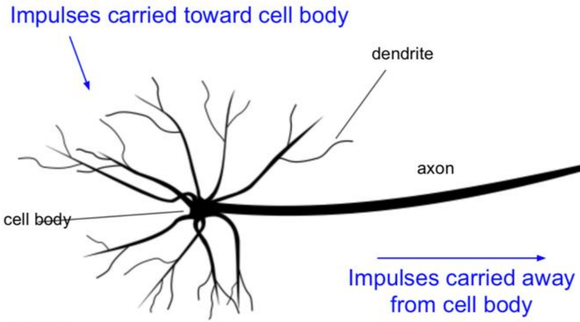
Some fun facts :

1 million x

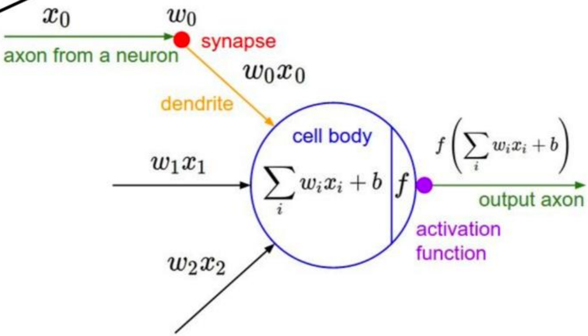
100 billion neurons

100,000 neurons

Multilayer Perceptrons

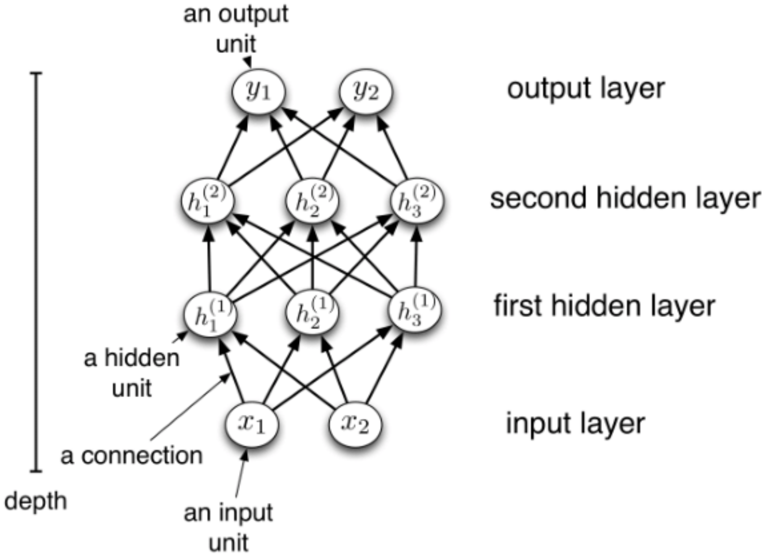

Impulses carried toward cell body
dendrite
presynaptic terminal
axon
cell body
Impulses carried away from cell body

This image by Felipe Perucho is licensed under CC-BY 3.0



Multilayer Perceptrons

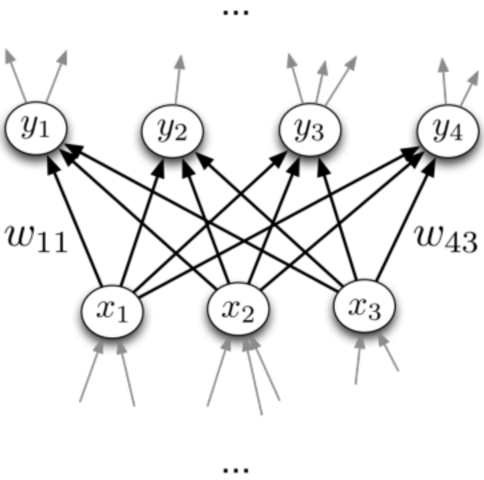
- We can connect lots of units together into a directed acyclic graph.
- This gives a feed-forward neural network. That's in contrast to recurrent neural networks, which can have cycles. (We'll talk about those later.)
- Typically, units are grouped together into layers.



Multilayer Perceptrons

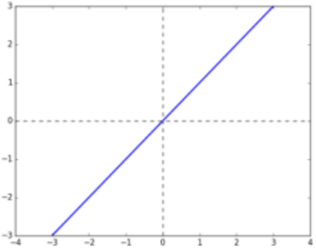
- Each layer connects N input units to M output units.
- In the simplest case, all input units are connected to all output units. We call this a fully connected layer. We'll consider other layer types later.
- Note: the inputs and outputs for a layer are distinct from the inputs and outputs to the network.

- Recall from softmax regression: this means we need an $M \times N$ weight matrix.
- The output units are a function of the input units:
$$\mathbf{y} = f(\mathbf{x}) = \phi\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right)$$
- A multilayer network consisting of fully connected layers is called a multilayer perceptron. Despite the name, it has nothing to do with perceptrons!



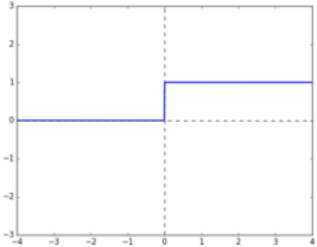
Multilayer Perceptrons

Some activation functions:



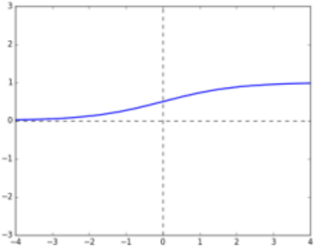
Linear

$$y = z$$



Hard Threshold

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

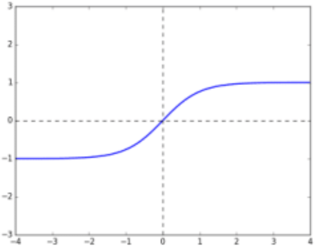


Logistic

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

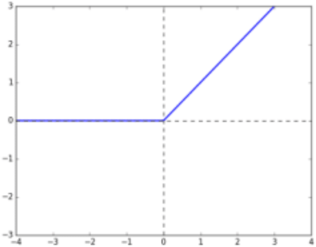
Multilayer Perceptrons

Some activation functions:



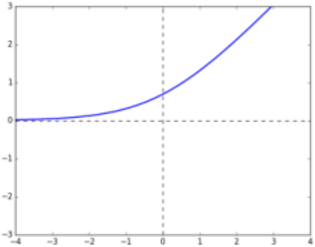
Hyperbolic Tangent (tanh)

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



Rectified Linear Unit (ReLU)

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



Soft ReLU

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

Multilayer Perceptrons

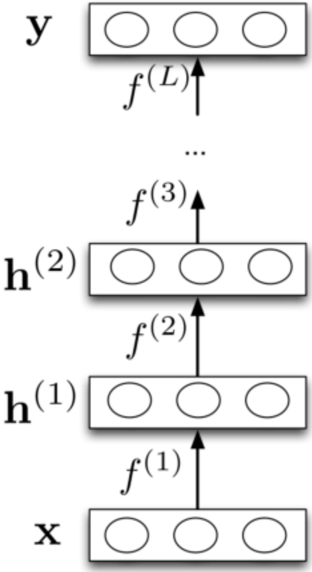
- Each layer computes a function, so the network computes a composition of functions:

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

- Or more simply:

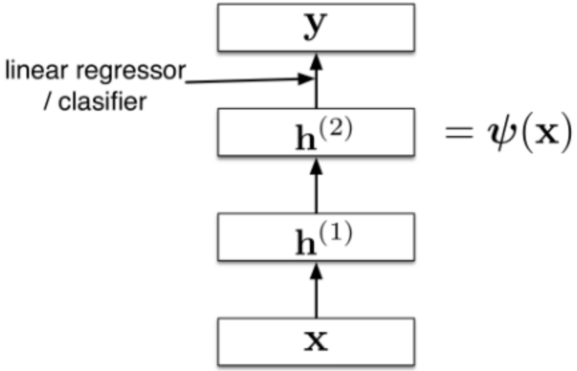
$$\mathbf{y} = f^{(L)} \circ \cdots \circ f^{(1)}(\mathbf{x}).$$

- 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:



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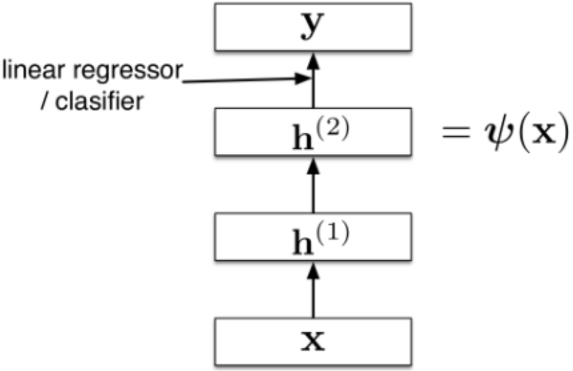
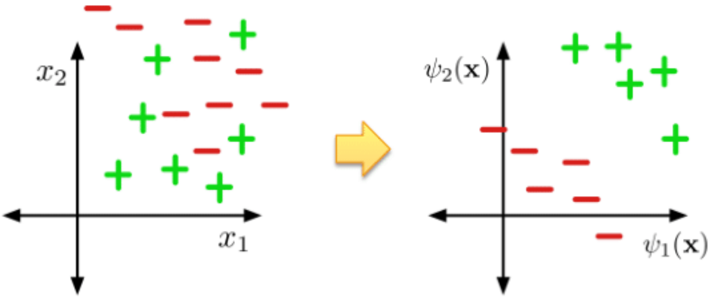


linear regressor / clasifier

- The goal:



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!

https://arxiv.org/pdf/1610.00291.pdf

Expressive Power

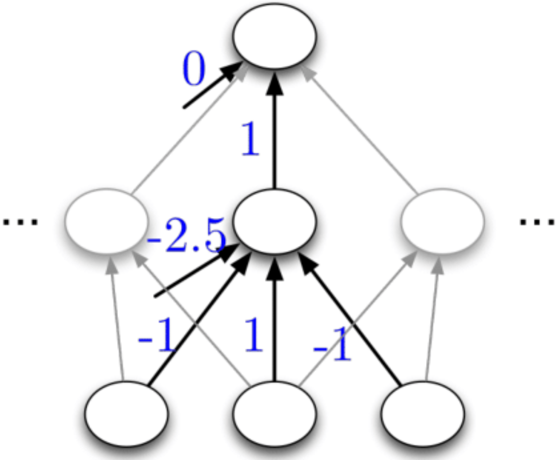
- Multilayer feed-forward neural nets with *nonlinear* activation functions are universal approximators: they can approximate any function arbitrarily well.
- This has been shown for various activation functions (thresholds, logistic, ReLU, etc.)
  - Even though ReLU is "almost" linear, it's nonlinear 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
	⋮		⋮
-1	-1	1	-1
-1	1	-1	1
-1	1	1	1
	⋮		⋮

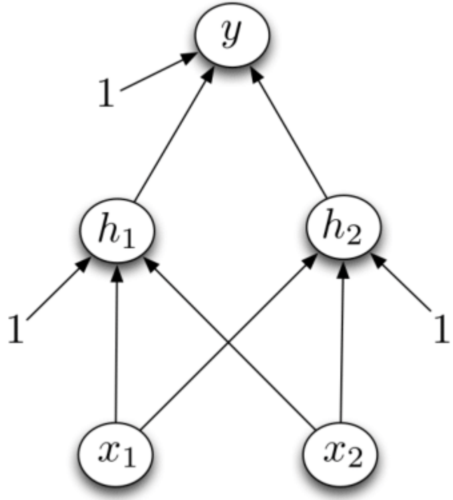


- Only requires one hidden layer, though it needs to be extremely wide!

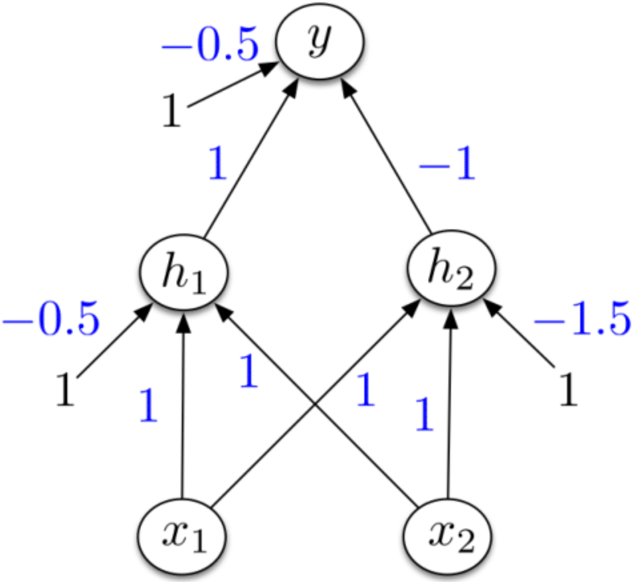
Multilayer Perceptrons

Designing a network to compute XOR:

Assume hard threshold activation function



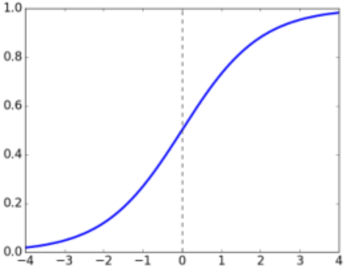
Multilayer Perceptrons



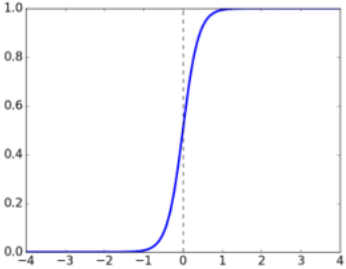
Exercise: Could you come up with another set of weights to compute XOR?

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 tune 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!

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

After the break

After the break: **Backpropagation**

After the break Back-Propagation

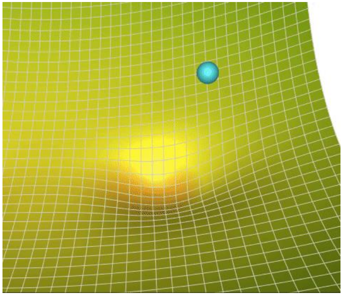
Source: https://www.youtube.com/watch?v=Suevq-kZdIw

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 $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$.

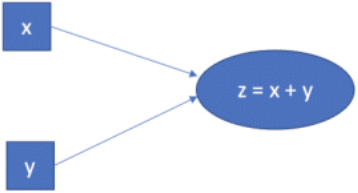
Recap : Univariate Chain Rule

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

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

Recap: Computation Graph

- A computational graph is a directed graph where the **nodes** correspond to **operations** or **variables**.
- Variables can feed their value into operations, and operations can feed their output into other operations. This way, every node in the graph defines a function of the variables.
- For example : we want to plot the operation $z = x + y$, then



Recap: Computation Graph

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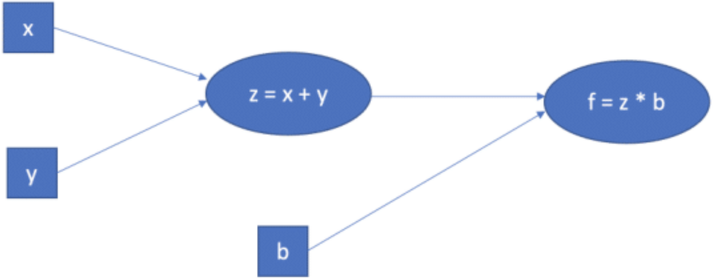
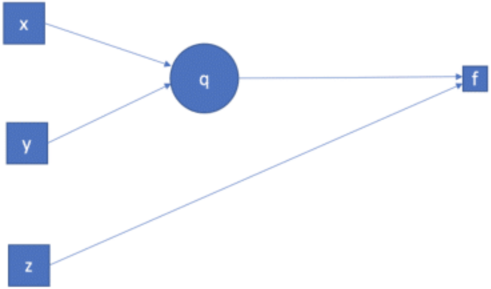
- Variables can feed their value into operations, and operations can feed their output into other operations. This way, every node in the graph defines a function of the variables.
- Another example : we want to plot the operation $f = (x + y) * b$, then



A simple example

$$f(x, y, z) = (x + y) * z$$

$$q = x + y; f = q * z$$



A simple example : Forward Pass

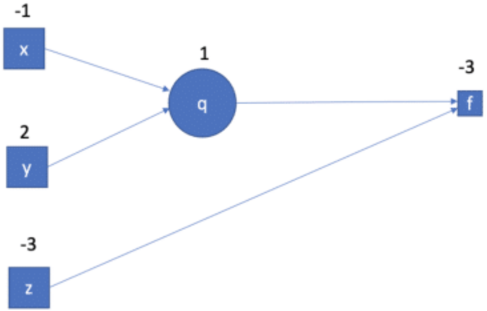
$$f(x, y, z) = (x + y) * z$$

$$q = x + y; f = q * z$$

$$e.g., x = -1, y = 2, z = 3$$

$$then, q = 1, f = -3$$

$$Want, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



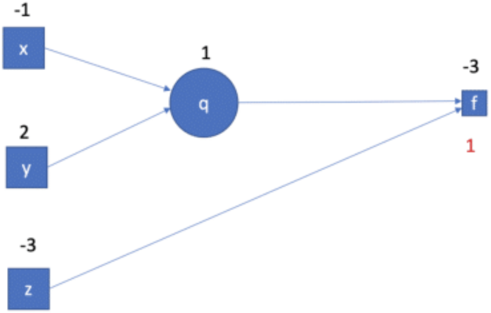
A simple example : Backward Pass

$$f(x, y, z) = (x + y) * z$$

$$q = x + y; f = q * z$$

$$e.g., x = -1, y = 2, z = 3$$

$$baseline : \frac{\partial f}{\partial f} = 1$$



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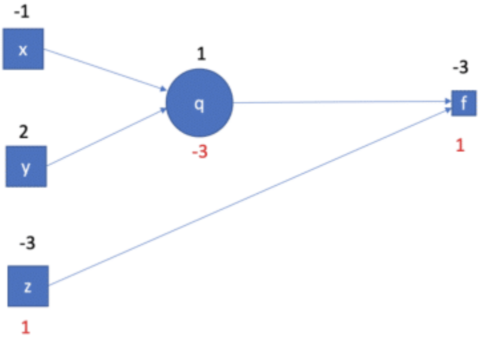
$$q = x+y; f = q*z$$

$$e.g., x = -1, y = 2, z = 3$$

$$baseline : \frac{\partial f}{\partial f} = 1$$

$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial z} = q = 1$$

$$\frac{\partial f}{\partial q} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial q} = z = -3$$



A simple example : Backward Pass

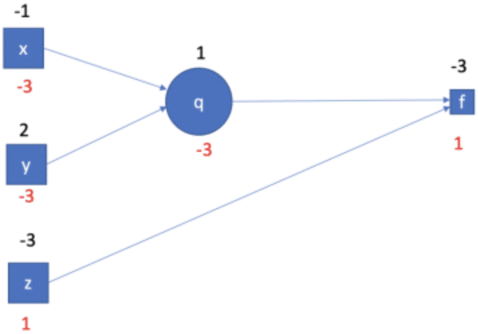
$$f(x, y, z) = (x + y) * z$$

$$q = x + y; f = q * z$$

$$e.g., x = -1, y = 2, z = 3$$

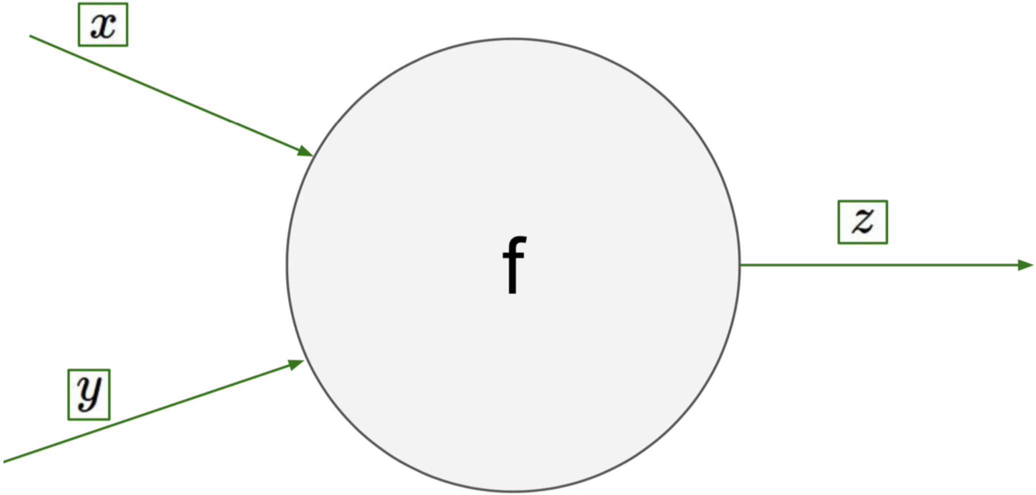
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} = (-3) * (1) = -3$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y} = (-3) * (1) = -3$$



A simple example : Backward Pass

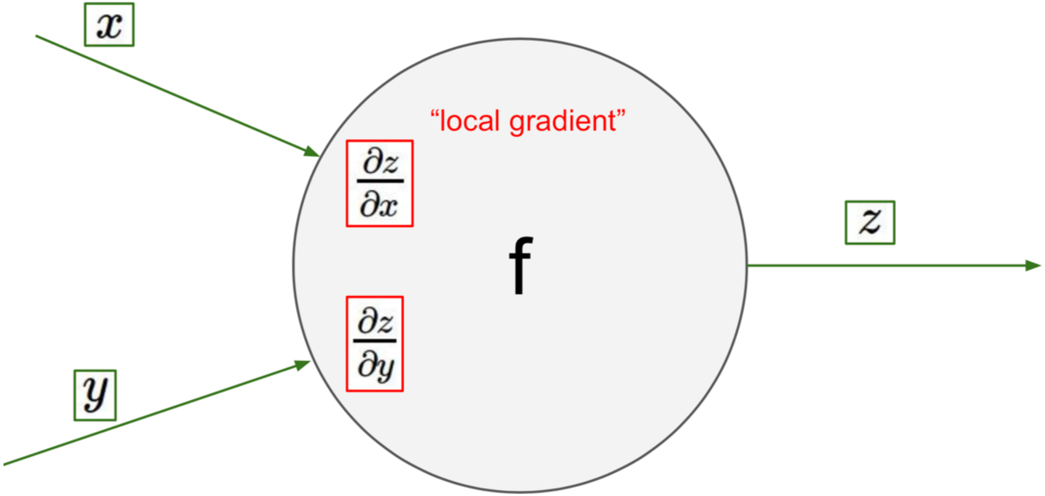
A quick summary:



Source: Fei-Fei Li & Justin Johnson & Serena Yeung, csc231N, Stanford University

A simple example : Backward Pass

A quick summary:

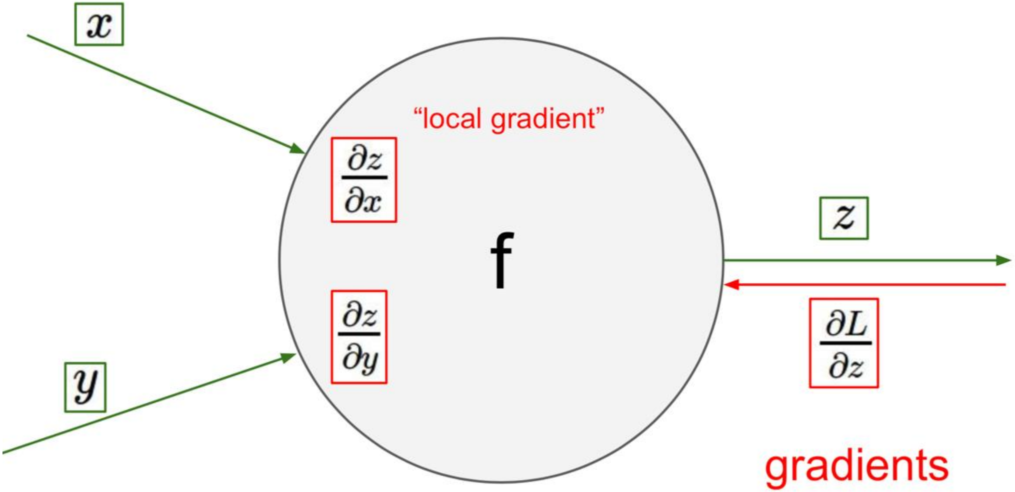


x
y
z
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f

Source: Fei-Fei Li & Justin Johnson & Serena Yeung, csc231N, Stanford University

A simple example : Backward Pass

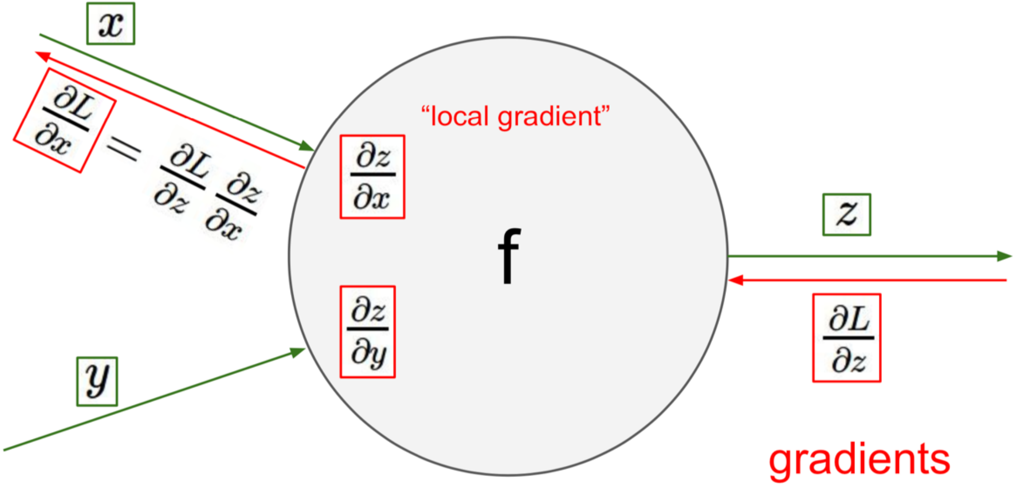
A quick summary:


x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
gradients

Source: Fei-Fei Li & Justin Johnson & Serena Yeung, csc231N, Stanford University

A simple example : Backward Pass

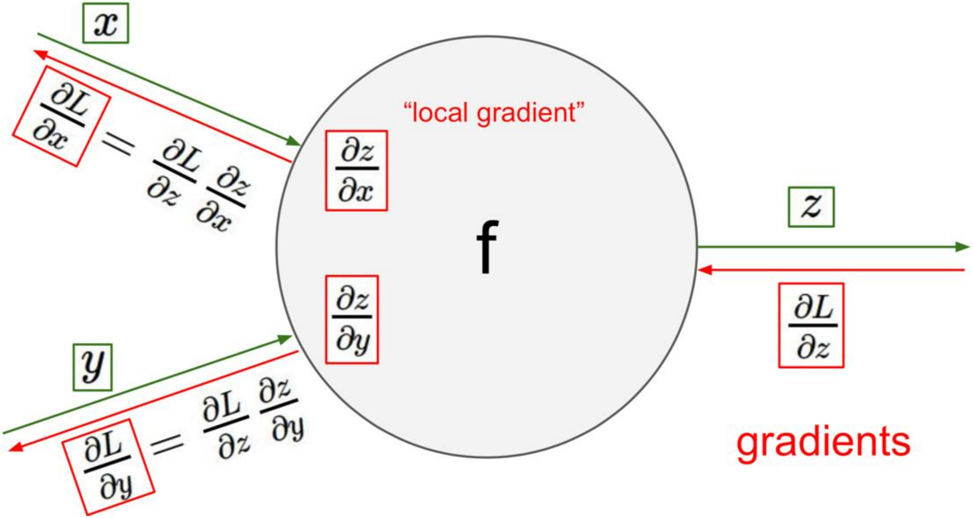
A quick summary:


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
y
z
$\frac{\partial L}{\partial z}$
gradients

Source: Fei-Fei Li & Justin Johnson & Serena Yeung, csc231N, Stanford University

A simple example : Backward Pass

A quick summary:



x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
z
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

Source: Fei-Fei Li & Justin Johnson & Serena Yeung, csc231N, Stanford University

A more complex example: logistic least squares model

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

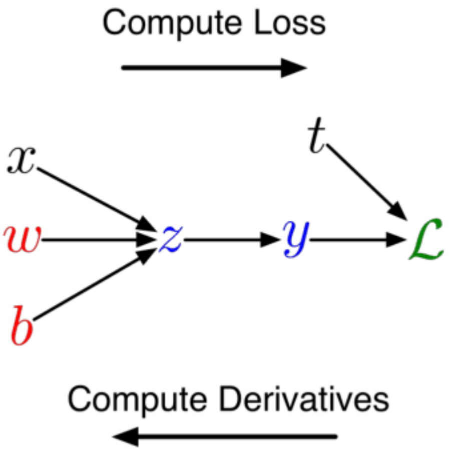
$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2}(\sigma(wx+b)-t)^2 \\
\frac{\partial \mathcal{L}}{\partial w} &= \frac{\partial}{\partial w}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial w}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial w}(\sigma(wx+b)-t)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

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

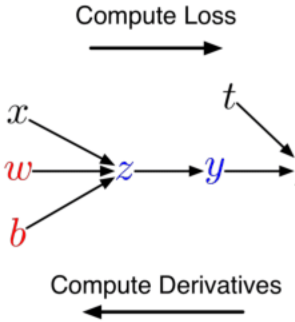
What are the disadvantages of this approach?

Univariate Chain Rule

- 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.



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:

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

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:

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

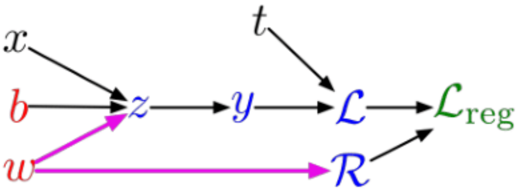
After the break

After the break: **Back-propagation in Multivariate Forms**

Multivariate Chain Rule

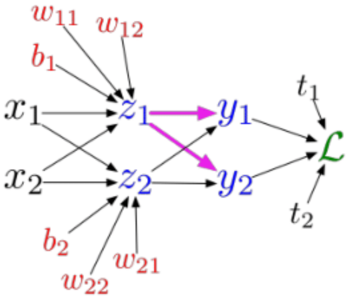
Problem: what if the computation graph has fan-out > 1?
This requires the multivariate Chain Rule!

L_2-Regularized regression



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

Multiclass logistic regression

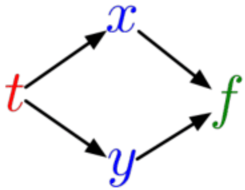


$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$
$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$
$$\mathcal{L} = -\sum_k t_k \log y_k$$

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:

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

- Plug in to Chain Rule:

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

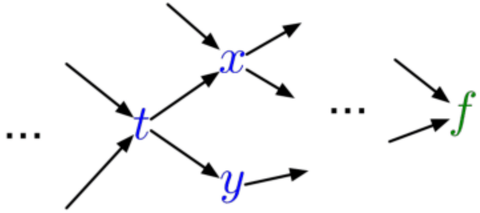
Multivariable Chain Rule

- 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

Full backpropagation algorithm:

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

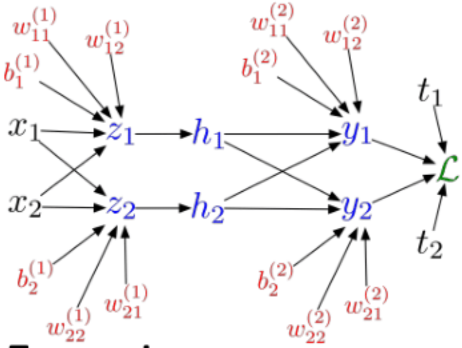
v_N denotes the variable we're trying to compute derivatives of (e.g. loss).

```
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

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:

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

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

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

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

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

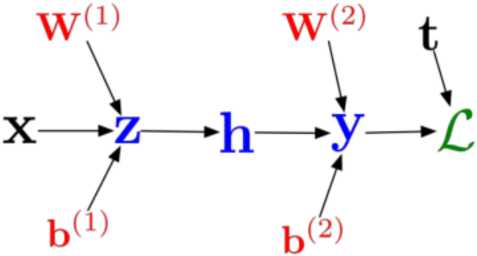
$$\overline{z_i} = \overline{h_i}\,\sigma'(z_i)$$

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

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

Vector Form

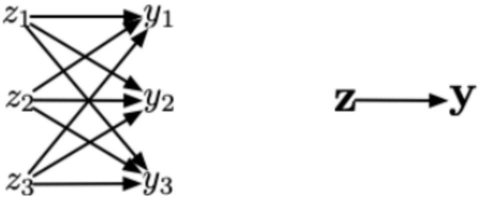
- Computation graphs showing individual units are cumbersome.
- As you might have guessed, we typically draw graphs over the vectorized variables.



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

Vector Form

- Consider this computation graph:



- Backprop rules:

$$\mathbf{z} \in \mathcal{R}^N, \mathbf{y} \in \mathcal{R}^M \qquad \overline{z_j} = \sum_k \overline{y_k} \frac{\partial y_k}{\partial z_j} \qquad \overline{\mathbf{z}} = \frac{\partial \mathbf{y}}{\partial \mathbf{z}}^\top \overline{\mathbf{y}},$$

where $\partial \mathbf{y}/\partial \mathbf{z}$ is the Jacobian matrix (**note**: check the matrix shapes):

$$(\frac{\partial \mathbf{y}}{\partial \mathbf{z}})_{M \times N} = \begin{pmatrix} \frac{\partial y_1}{\partial z_1} & \cdots & \frac{\partial y_1}{\partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial z_1} & \cdots & \frac{\partial y_m}{\partial z_n} \end{pmatrix}$$

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 (VJP) directly.

Hessian: Higher-order Gradients

- Hessian

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 \mathcal{L}}{\partial x_1^2} & \frac{\partial^2 \mathcal{L}}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 \mathcal{L}}{\partial x_1 \partial x_n} \\ \frac{\partial^2 \mathcal{L}}{\partial x_2 \partial x_1} & \frac{\partial^2 \mathcal{L}}{\partial x_2^2} & \cdots & \frac{\partial^2 \mathcal{L}}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 \mathcal{L}}{\partial x_n \partial x_1} & \frac{\partial^2 \mathcal{L}}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 \mathcal{L}}{\partial x_n^2} \end{pmatrix}$$

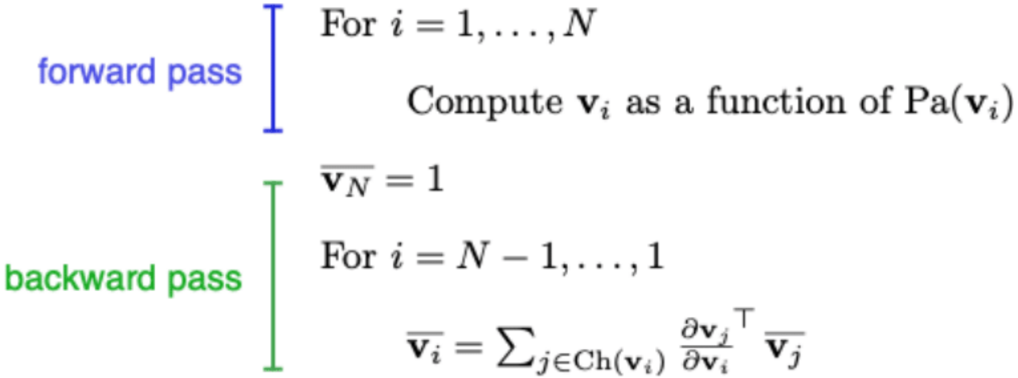
- Note: Again, we never explicitly construct the Hessian. It's usually simpler and more efficient to compute the Vector Hessian Product (VHP) directly.
- Note: You will need to practice this in HW1.

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.)

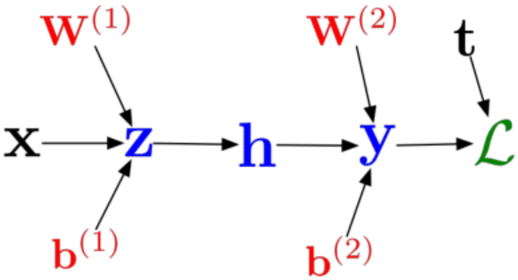
$\mathbf{v}_N$ denotes the variable we're trying to compute derivatives of (e.g. loss). It's a scalar, which we can treat as a 1-D vector.


forward pass
backward pass

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

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

The psychological profiling [of a programmer] is mostly the ability to shift levels of abstraction, from low level to high level. To see something in the small and to see something in the large.

– Don Knuth

- 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!