CSC413/2516 Lecture 2: Multilayer Perceptrons & Backpropagation

Jimmy Ba

- 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.

Convex Sets



• A set S is convex if any line segment connecting points in S lies entirely within S. Mathematically,

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

A simple inductive argument shows that for x₁,..., x_N ∈ S, weighted averages, or convex combinations, lie within the set:

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

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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!

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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!

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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, ..., 0.25). Therefore, this point must be classified as A.
- Similarly, the average of all translations of B is also (0.25, 0.25, ..., 0.25). Therefore, it must be classified as B. Contradiction!

Image: A market of the second seco

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

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

$$\frac{x_1 \quad x_2}{0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0}$$

$$\frac{x_1 \quad x_2}{0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0}$$

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- 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.

- 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.



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- 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!



Some activation functions:



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Some activation functions:



Designing a network to compute XOR:

Assume hard threshold activation function





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

$$h^{(1)} = f^{(1)}(\mathbf{x})$$

$$h^{(2)} = f^{(2)}(\mathbf{h}^{(1)})$$

$$\vdots$$

$$\mathbf{y} = f^{(L)}(\mathbf{h}^{(L-1)})$$

• 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.

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



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



Input representation of a digit : 784 dimensional vector.

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- Each first-layer hidden unit computes $\sigma(\mathbf{w}_i^T \mathbf{x})$
- Here is one of the weight vectors (also called a feature).
- It's reshaped into an image, with gray = 0, white = +, black = -.
- To compute $\mathbf{w}_i^T \mathbf{x}$, multiply the corresponding pixels, and sum the result.



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There are 256 first-level features total. Here are some of them.

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- 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!

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- Multilayer feed-forward neural nets with *nonlinear* activation functions are <u>universal approximators</u>: 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!

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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



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

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



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

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• Limits of universality

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- 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!

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- 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

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After the break

After the break: Backpropagation

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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.

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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 ${\rm d}\mathcal{J}/{\rm d}\boldsymbol{w},$ which is the vector of partial derivatives.
 - This is the average of $d\mathcal{L}/d\mathbf{w}$ over all the training examples, so in this lecture we focus on computing $d\mathcal{L}/d\mathbf{w}$.

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

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

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Recall: Univariate logistic least squares model

$$z = wx + b$$

$$y = \sigma(z)$$

$$\mathcal{L} = \frac{1}{2}(y - t)^{2}$$

Let's compute the loss derivatives.

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How you would have done it in calculus class

$$\mathcal{L} = \frac{1}{2} (\sigma(wx+b)-t)^2$$

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

$$= \frac{1}{2} \frac{\partial}{\partial w} (\sigma(wx+b)-t)^2$$

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

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

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

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

$$= (\sigma(wx+b)-t) \sigma'(wx+b) x$$

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

$$= \frac{1}{2} \frac{\partial}{\partial b} (\sigma(wx+b)-t)^2$$

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

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

$$= (\sigma(wx+b)-t) \sigma'(wx+b) x$$

What are the disadvantages of this approach?

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A more structured way to do it

Computing the derivatives:

Computing the loss: z = wx + b $y = \sigma(z)$ $\mathcal{L} = \frac{1}{2}(y - t)^{2}$ $\frac{d\mathcal{L}}{dy} = y - t$ $\frac{d\mathcal{L}}{dz} = \frac{d\mathcal{L}}{dy} \sigma'(z)$ $\frac{\partial\mathcal{L}}{\partial w} = \frac{d\mathcal{L}}{dz} \times$ $\frac{\partial\mathcal{L}}{\partial b} = \frac{d\mathcal{L}}{dz}$

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

- 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.



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A slightly more convenient notation:

- Use \overline{y} to denote the derivative $d\mathcal{L}/dy$, 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:

Computing the derivatives:

 $z = wx + b \qquad \qquad \overline{y} = y - t$ $y = \sigma(z) \qquad \qquad \overline{z} = \overline{y} \sigma'(z)$ $\mathcal{L} = \frac{1}{2}(y - t)^2 \qquad \qquad \overline{w} = \overline{z} x$ $\overline{b} = \overline{z}$

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Multivariate Chain Rule

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



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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:

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

Multivariable Chain Rule

• In the context of backpropagation:



In our notation:

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

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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).

Backpropagation

Example: univariate logistic least squares regression



Forward pass:



Backward pass:

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

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Backpropagation

Multilayer Perceptron (multiple outputs):



Forward pass:

$$egin{aligned} & z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)} \ & h_i = \sigma(z_i) \ & y_k = \sum_i w_{ki}^{(2)} h_i + b_k^{(2)} \ & \mathcal{L} = rac{1}{2} \sum_k (y_k - t_k)^2 \end{aligned}$$

Backward pass:

$$\begin{split} \overline{\mathcal{L}} &= 1\\ \overline{y_k} &= \overline{\mathcal{L}} \left(y_k - t_k \right)\\ \overline{w_{ki}^{(2)}} &= \overline{y_k} h_i\\ \overline{b_k^{(2)}} &= \overline{y_k}\\ \overline{h_i} &= \sum_k \overline{y_k} w_{ki}^{(2)}\\ \overline{z_i} &= \overline{h_i} \sigma'(z_i)\\ \overline{w_{ij}^{(1)}} &= \overline{z_i} x_j\\ \overline{b_i^{(1)}} &= \overline{z_i} \end{split}$$

- 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.

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• Consider this computation graph:



• Backprop rules:

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

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

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

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Examples

Matrix-vector product

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

• Elementwise operations

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

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

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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
$$\begin{bmatrix} & \text{For } i = 1, \dots, N \\ & \text{Compute } \mathbf{v}_i \text{ as a function of } Pa(\mathbf{v}_i \\ & \overline{\mathbf{v}_N} = 1 \\ & \text{For } i = N - 1, \dots, 1 \\ & \overline{\mathbf{v}_i} = \sum_{j \in Ch(\mathbf{v}_i)} \frac{\partial \mathbf{v}_j}{\partial \mathbf{v}_i}^\top \overline{\mathbf{v}_j} \end{bmatrix}$$

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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:

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

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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

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

 Rule of thumb: the backward pass is about as expensive as two forward passes.

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• 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?

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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

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- 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!