

Lecture 3: Neural Networks

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Deep Structured Learning Course, Fall 2019

Announcements

Homework 1's deadline is October 11 (next week)

Deadline for project proposal: October 18 (two weeks from now)

- List of project ideas will be put soon in the course webpage!
- You need to turn in a 1-page proposal (use NIPS format) explaining:
 - The problem you propose to solve
 - Which method(s) you are going to use
 - Which evaluation metric and which data you are going to use
- Team size: 2–3 people

Announcements

Next week: We will have a guest lecture!

- The lecture will be a practical Pytorch tutorial
- Please bring your laptops if you can!
- Even better: install Pytorch in your computer before the lecture!

Today's Roadmap

Today's lecture is about **neural networks**:

- From perceptron to multi-layer perceptron
- Feed-forward neural networks
- Activation functions: sigmoid, tanh, relu, ...
- Activation maps: softmax, sparsemax, ...
- Non-convex optimization and local minima
- Universal approximation theorem
- Gradient backpropagation

Outline

① Neural Networks

Definition

Activations

Feed-forward Neural Networks

Universal Approximation

② Training Neural Networks

Empirical Risk Minimization

Gradient Backpropagation

Tricks of the Trade

③ Conclusions

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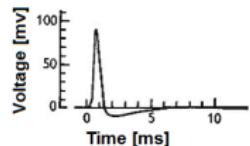
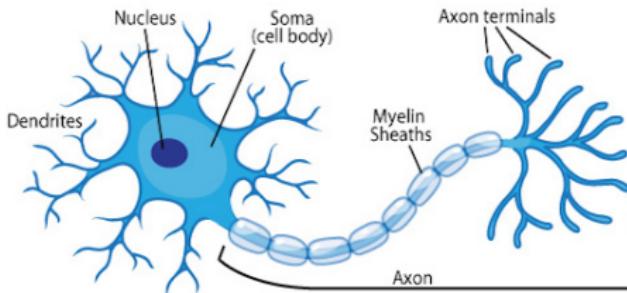
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Gradient Backpropagation

Tricks of the Trade

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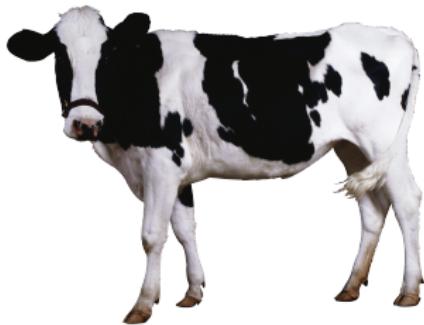
Biological Neuron



- Three main parts: the main body (**soma**), **dendrites** and an **axon**
- The neuron receives input signals from dendrites, and then outputs its own signals through the axon
- Axons in turn connect to the dendrites of other neurons, using special connections called **synapses**
- Generate sharp electrical potentials across their cell membrane (**spikes**), a major signaling unit of the nervous system

Word of Caution

- Artificial neurons are inspired by biological neurons in nervous systems, but...



Warren McCulloch and Walter Pitts



- The earliest computational model of a neuron, via **threshold logic** (McCulloch and Pitts, 1943).

Artificial Neuron (McCulloch and Pitts, 1943)

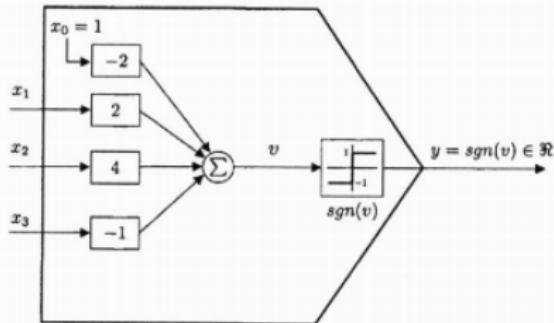


Figure 3.6 Example 3.2: a threshold neural logic for $y = x_2(x_1 + \bar{x}_3)$.

Table 3.6 Truth table for Example 3.2

Neural Inputs			$v = \mathbf{w}_a^T \mathbf{x}_a$ $= -2 + 2x_1 + 4x_2 - x_3$	$y = sgn(v)$ $= sgn(\mathbf{w}_a^T \mathbf{x}_a)$
-1	-1	-1	-7	-1
-1	-1	1	-9	-1
-1	1	-1	1	1
-1	1	1	-1	-1
1	-1	-1	-3	-1
1	-1	1	-5	-1
1	1	-1	5	1
1	1	1	3	1

- Later models replaced the hard threshold by more general activations

Artificial Neuron

- **Pre-activation** (input activation):

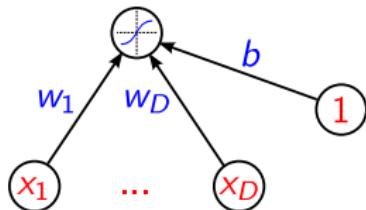
$$z(x) = \mathbf{w} \cdot \mathbf{x} + b = \sum_{i=1}^D w_i x_i + b,$$

where \mathbf{w} are the **connection weights** and b is a **bias term**.

- **Activation:**

$$h(x) = g(z(x)) = g(\mathbf{w} \cdot \mathbf{x} + b),$$

where $g : \mathbb{R} \rightarrow \mathbb{R}$ is the **activation function**.



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Activation Function

Typical choices:

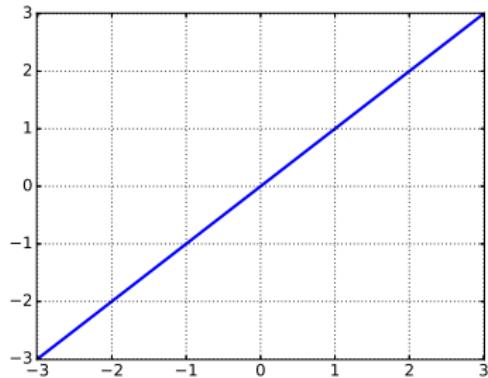
- Linear
- Sigmoid (logistic function)
- Hyperbolic Tangent
- Rectified Linear

Later:

- Softmax
- Sparsemax
- Max-pooling

Linear Activation

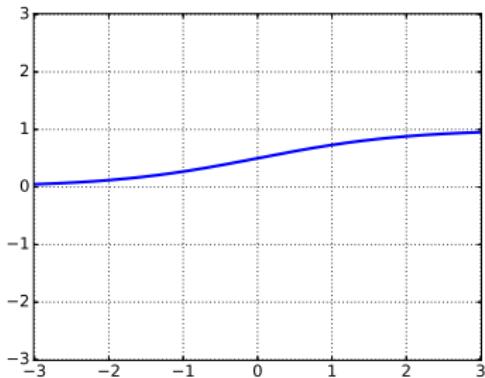
$$g(z) = z$$



- No “squashing” of the input
- Composing layers of linear units is equivalent to a single layer of linear units, so no expressive power added when going multi-layer (more later)
- Still useful to linear-project the input to a lower dimension

Sigmoid Activation

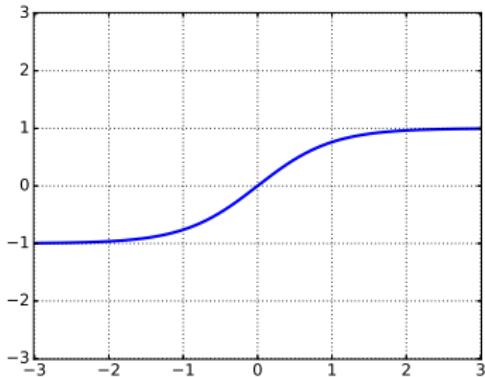
$$g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}$$



- “Squashes” the neuron pre-activation between 0 and 1
- The output can be interpreted as a probability
- Positive, bounded, strictly increasing
- Logistic regression corresponds to a network with a single sigmoid unit
- Combining layers of sigmoid units will increase expressiveness (more later)

Hyperbolic Tangent Activation

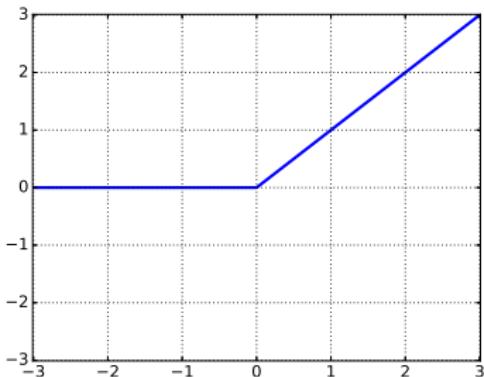
$$g(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$



- “Squashes” the neuron pre-activation between -1 and 1
- Related to the sigmoid via $\sigma(z) = \frac{1+\tanh(z/2)}{2}$
- Can be positive or negative, bounded, strictly increasing
- Combining layers of tanh units will increase expressiveness (more later)

Rectified Linear Unit Activation (Glorot et al., 2011)

$$g(z) = \text{relu}(z) = \max\{0, z\}$$



- Less prone to vanishing gradients (more later), and historically the first activation that allowed training deep nets without unsupervised pre-training (Glorot et al., 2011)
- Non-negative, increasing, **but not upper bounded**
- Not differentiable at 0
- Leads to neurons with **sparse activities** (biologically more plausible)

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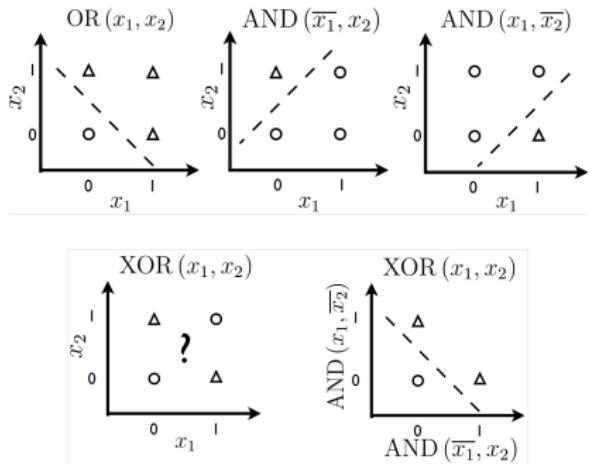
③ Conclusions

Capacity of Single Neuron (Linear Classifier)

- With a single sigmoid activated neuron we recover **logistic regression**:

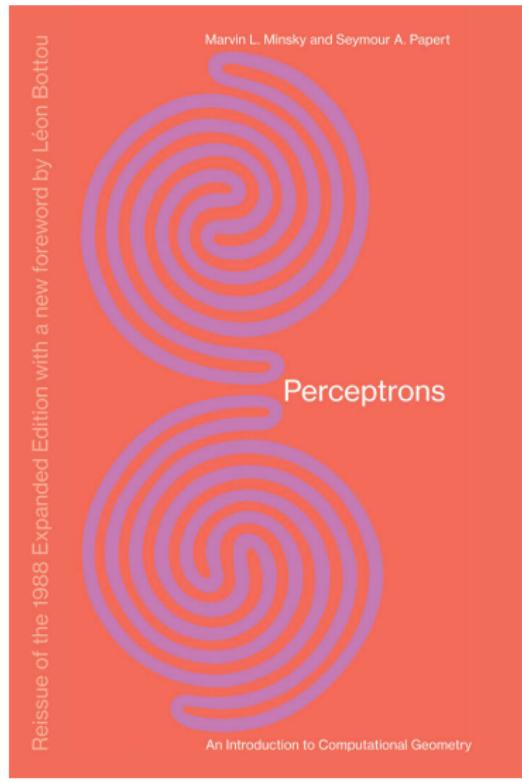
$$p(y = 1|x) = \sigma(\mathbf{w} \cdot \mathbf{x} + b).$$

- Can solve linearly separable problems (OR, AND)
- Can't solve non-linearly separable problems (XOR)—unless input is transformed into a better representation



(Slide credit: Hugo Larochelle)

The XOR Affair



Minsky and Papert (1969):

- Misunderstood by many as showing a single perceptron cannot learn XOR (in fact, this was already well-known at the time)
- Fostered an “AI winter” period

Solving XOR with Multi-Layer Perceptron

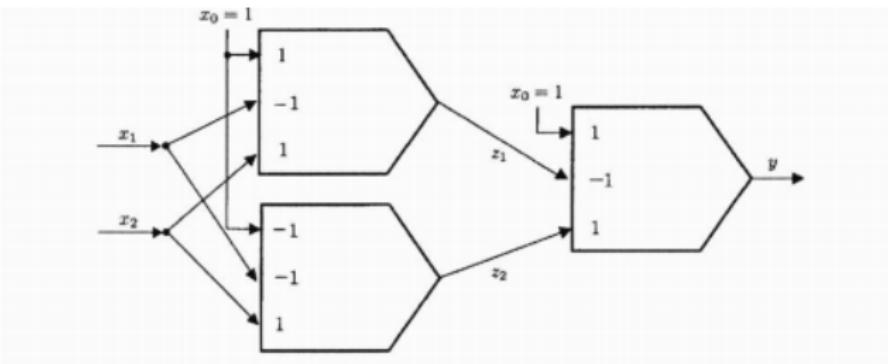


Figure 3.11 Example 3.6: a threshold network for XOR function $y = x_1 \oplus x_2 = sgn(1 - z_1 + z_2)$, $z_1 = sgn(1 - x_1 + x_2)$, $z_2 = sgn(-1 - x_1 + x_2)$.

Solving XOR with Multi-Layer Perceptron

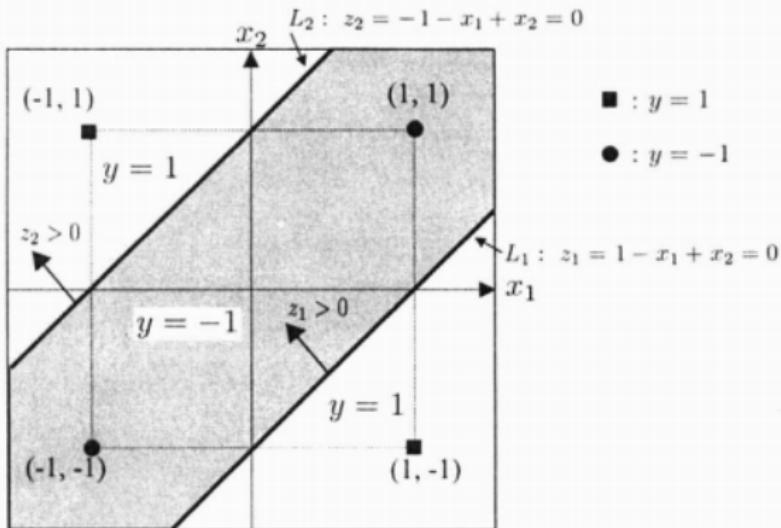


Figure 3.12 Example 3.6: two discriminant lines for XOR function $y = x_1 \oplus x_2$.

Solving XOR with Multi-Layer Perceptron

- This construction was known by McCulloch and Pitts themselves!
- The negative result in Minsky and Papert (1969) is that, to learn arbitrary logic functions, each hidden unit needs to be connected to **all inputs**
- At the time, there was some hope that we'd only need “local” neurons

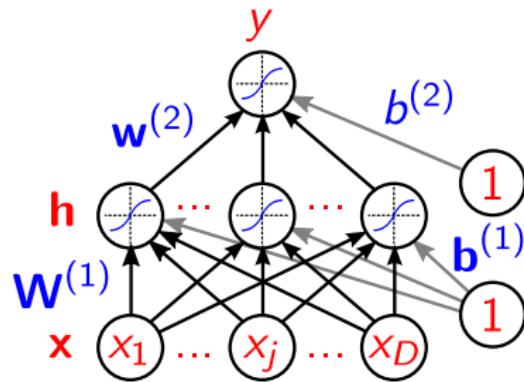
Multi-Layer Neural Network

- **Key idea:** add intermediate layers of artificial neurons before the final output layer
- Each of these hidden units computes some representation of the input and propagates forward that representation
- This increases the expressive power of the network, yielding more complex, non-linear, classifiers
- Similar role as latent variables in probabilistic models, but no need for a probability semantics
- Also called **feed-forward neural network**

Single Hidden Layer

To start simple, let's assume our task involves several inputs ($x \in \mathbb{R}^D$) but a **single output** (e.g. $y \in \mathbb{R}$ or $y \in \{0, 1\}$)

Trick: add an intermediate layer of K hidden units ($h \in \mathbb{R}^K$)



Single Hidden Layer

Assume D inputs ($x \in \mathbb{R}^D$) and K hidden units ($h \in \mathbb{R}^K$)

- **Hidden layer pre-activation:**

$$z(x) = \mathbf{W}^{(1)}x + \mathbf{b}^{(1)},$$

with $\mathbf{W}^{(1)} \in \mathbb{R}^{K \times D}$ and $\mathbf{b}^{(1)} \in \mathbb{R}^K$.

- **Hidden layer activation:**

$$h(z) = g(z(x)),$$

where $g : \mathbb{R}^K \rightarrow \mathbb{R}^K$ is applied vectorwise.

- **Output layer activation:**

$$f(x) = o(\mathbf{w}^{(2)} \cdot h + b^{(2)}),$$

where $\mathbf{w}^{(2)} \in \mathbb{R}^K$ and $o : \mathbb{R} \rightarrow \mathbb{R}$ if the output activation function.

Single Hidden Layer

Overall,

$$\begin{aligned}f(\mathbf{x}) &= o(\mathbf{w}^{(2)} \cdot \mathbf{h} + b^{(2)}) \\&= o(\mathbf{w}^{(2)} \cdot \mathbf{g}(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) + b^{(2)})\end{aligned}$$

Examples:

- $o(u) = u$ for **regression** ($y \in \mathbb{R}$)
- $o(u) = \sigma(u)$ for **binary classification** ($y \in \{-1, +1\}$, $f(\mathbf{x}) = P(y | \mathbf{x})$)

No longer a **linear classifier** – non-linear dependency on $\mathbf{W}^{(1)}$ and $\mathbf{b}^{(1)}$

\mathbf{h} is a vector of **internal representations** (as opposed to manually engineered features)

Single Hidden Layer

Can we use a similar strategy for **multi-class classification**? What do we need to change?

Multiple Classes

For multi-class classification, we need **multiple output units** (one per class)

Each output estimates the conditional probability $p(y = c | \mathbf{x})$

Predicted class is the one with highest estimated probability

We'll see two activation functions suitable for this:

- Softmax activation
- Sparsemax activation

Softmax Activation

Let $\Delta^{C-1} \subseteq \mathbb{R}^C$ be the probability simplex

The typical activation function for multi-class classification is
softmax : $\mathbb{R}^C \rightarrow \Delta^{C-1}$:

$$\mathbf{o}(z) = \text{softmax}(z) = \left[\frac{\exp(z_1)}{\sum_c \exp(z_c)}, \dots, \frac{\exp(z_C)}{\sum_c \exp(z_c)} \right]$$

- We say this already in class, when talking about logistic regression!
- Strictly positive, sums to 1
- Resulting distribution has full support: $\text{softmax}(z) > \mathbf{0}, \forall z$
- A disadvantage if a *sparse* probability distribution is desired
- Common workaround: threshold and truncate

Sparsemax Activation (Martins and Astudillo, 2016)

A sparse-friendly alternative is **sparsemax** : $\mathbb{R}^C \rightarrow \Delta^{C-1}$, defined as:

$$\mathbf{o}(z) = \text{sparsemax}(z) := \arg \min_{\mathbf{p} \in \Delta^{C-1}} \|\mathbf{p} - z\|^2.$$

- In words: Euclidean projection of z onto the probability simplex
- Likely to hit the boundary of the simplex, in which case $\text{sparsemax}(z)$ becomes sparse (hence the name)
- Retains many of the properties of softmax (e.g. differentiability), having in addition the ability of producing sparse distributions
- Projecting onto the simplex amounts to a **soft-thresholding** operation (next)
- Efficient forward/backward propagation (more later)

Sparsemax in Closed Form

- Projecting onto the simplex amounts to a soft-thresholding operation:

$$\text{sparsemax}_i(\mathbf{z}) = \max\{0, z_i - \tau\}$$

where τ is a normalizing constant such that $\sum_j \max\{0, z_j - \tau\} = 1$

- To evaluate the sparsemax, all we need is to compute τ
- Coordinates above the threshold will be shifted by this amount; the others will be truncated to zero

A Formal Algorithm

Input: $\mathbf{z} \in \mathbb{R}^C$

Sort \mathbf{z} as $z_{(1)} \geq \dots \geq z_{(C)}$

Find $k(\mathbf{z}) := \max \left\{ k \in [C] \mid 1 + kz_{(k)} > \sum_{j \leq k} z_{(j)} \right\}$

Define $\tau(\mathbf{z}) = \frac{(\sum_{j \leq k(\mathbf{z})} z_{(j)}) - 1}{k(\mathbf{z})}$

Output: $\mathbf{p} \in \Delta^{C-1}$ s.t. $p_i = [z_i - \tau(\mathbf{z})]_+$.

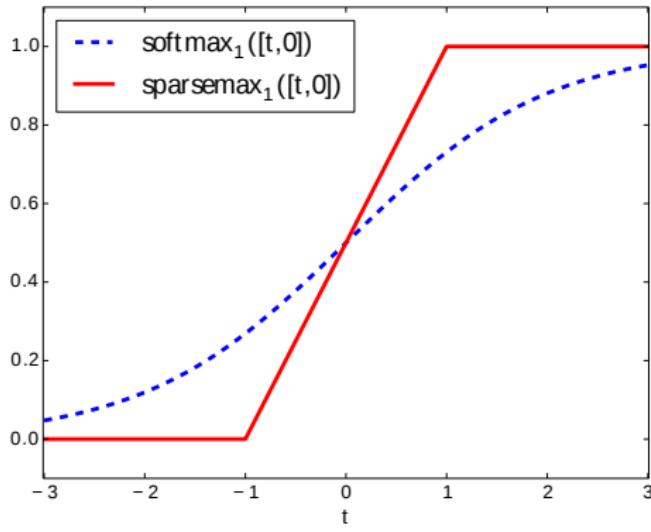
- Time complexity is $O(C \log C)$ due to the sort operation; but $O(C)$ algorithms exist based on linear-time selection.
- Note: evaluating **softmax** costs $O(C)$ too.

Two Dimensions

- Parametrize $z = (t, 0)$
- The 2D **softmax** is the logistic (sigmoid) function:

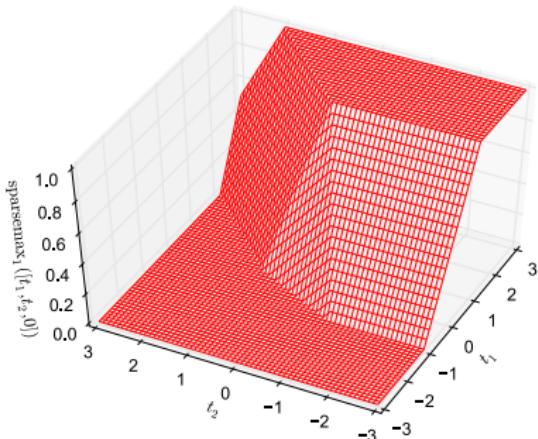
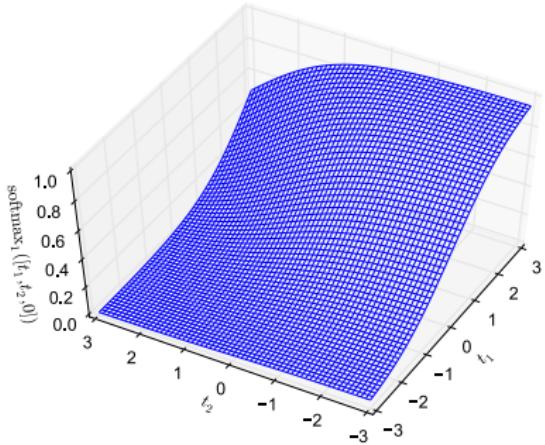
$$\text{softmax}_1(z) = (1 + \exp(-t))^{-1}$$

- The 2D **sparsemax** is the “hard” version of the sigmoid:



Three Dimensions

- Parameterize $z = (t_1, t_2, 0)$ and plot **softmax**₁(z) and **sparsemax**₁(z) as a function of t_1 and t_2
- **sparsemax** is piecewise linear, but asymptotically similar to **softmax**



Multi-Layer Neural Networks: General Case

In general we can:

- Have multiple output units (needed for multi-class classification)
- Stack more layers on top of each other

Multiple Hidden Layers

Now assume $L \geq 1$ hidden layers:

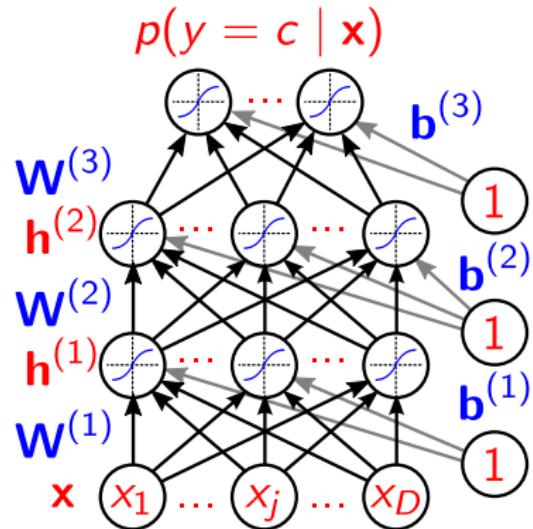
- **Hidden layer pre-activation** (define $h^{(0)} = x$ for convenience):

$$z^{(\ell)}(x) = \mathbf{W}^{(\ell)} h^{(\ell-1)} + \mathbf{b}^{(\ell)},$$

with $\mathbf{W}^{(\ell)} \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$ and $\mathbf{b}^{(\ell)} \in \mathbb{R}^{K_\ell}$.

- **Hidden layer activation:**

$$h^{(\ell)}(x) = g(z^{(\ell)}(x)).$$



- **Output layer activation:**

$$f(x) = o(z^{(L+1)}(x)) = o(\mathbf{W}^{(L+1)} h^{(L)} + \mathbf{b}^{(L+1)}).$$

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Universal Approximation Theorem

Theorem (Hornik et al. (1989))

A neural network with a single hidden layer and a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units.

- First proved for the sigmoid case by Cybenko (1989), then to **tanh** and many other activation functions by Hornik et al. (1989)
- **Caveat:** may need exponentially many hidden units

Deeper Networks

- **Deeper networks** (more hidden layers) can provide more compact approximations

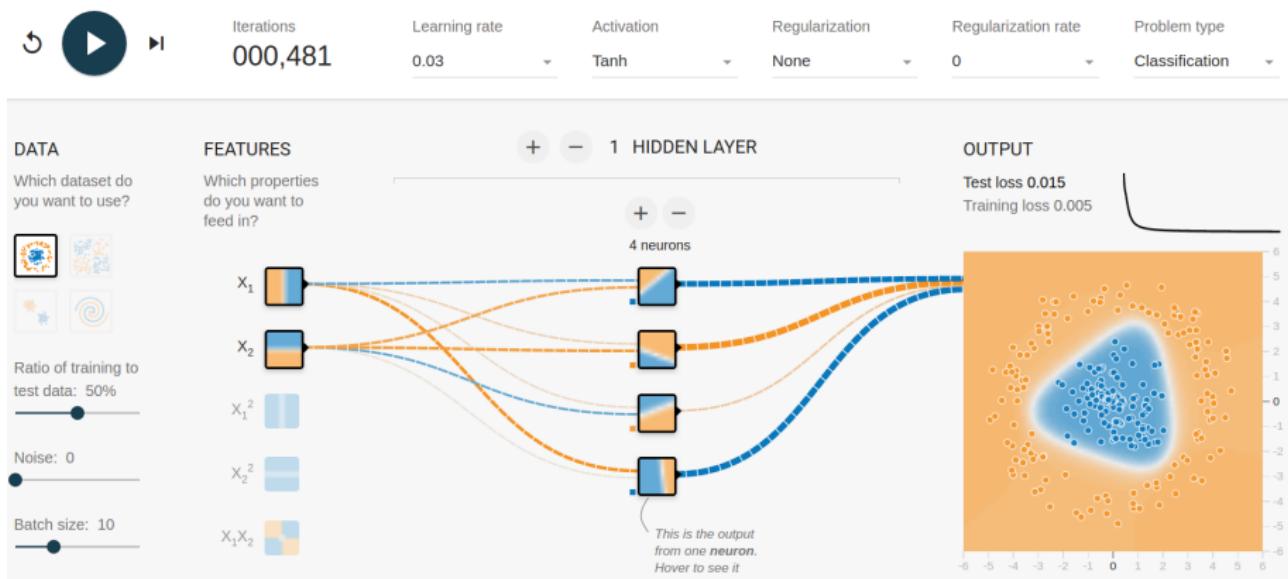
Theorem (Montufar et al. (2014))

The number of linear regions carved out by a deep neural network with D inputs, depth L , and K hidden units per layer with ReLU activations is

$$O\left(\left(\frac{K}{D}\right)^{D(L-1)} K^D\right)$$

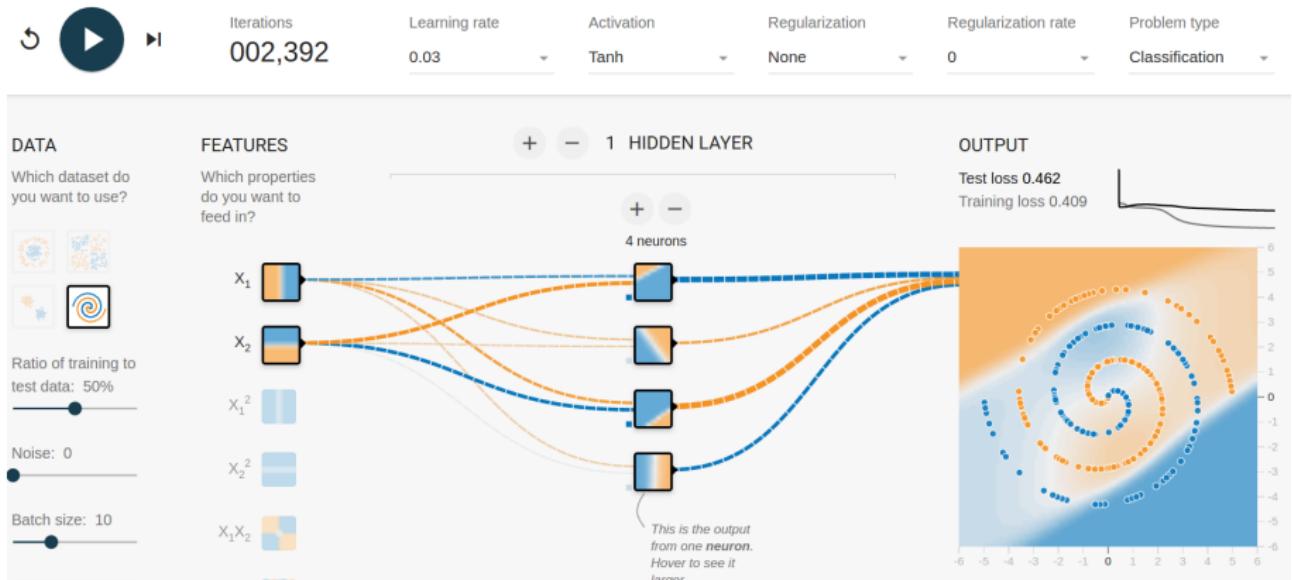
Therefore, for fixed K , deeper networks are exponentially more expressive

“Simple” Target Function, One Hidden Layer



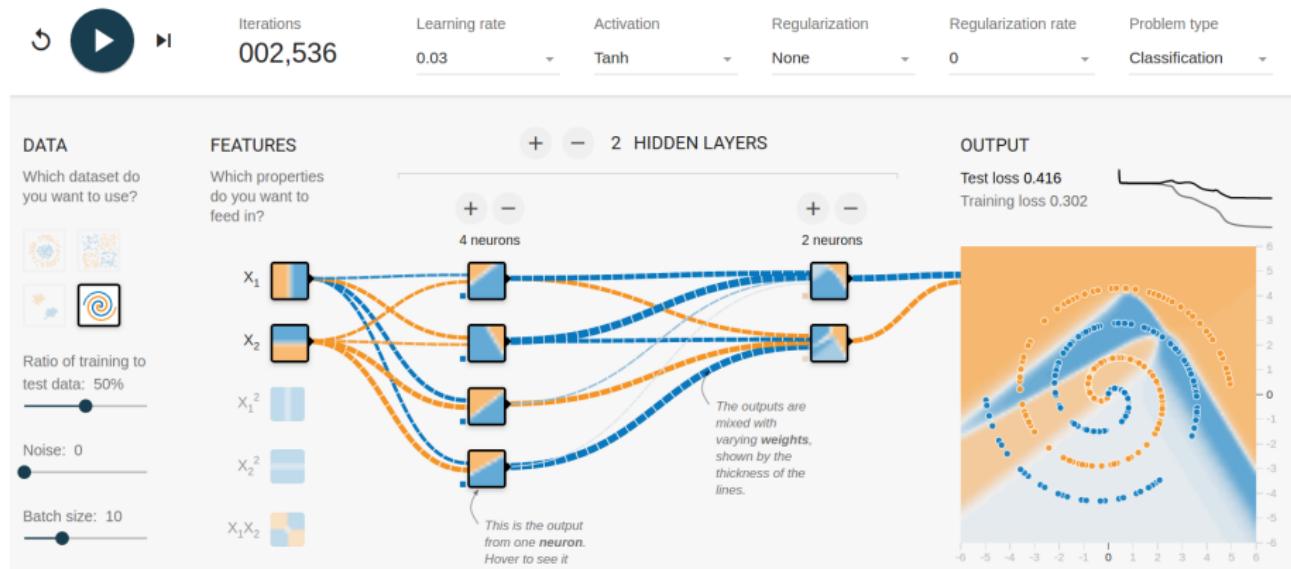
(<http://playground.tensorflow.org>)

Complex Target Function, One Hidden Layer



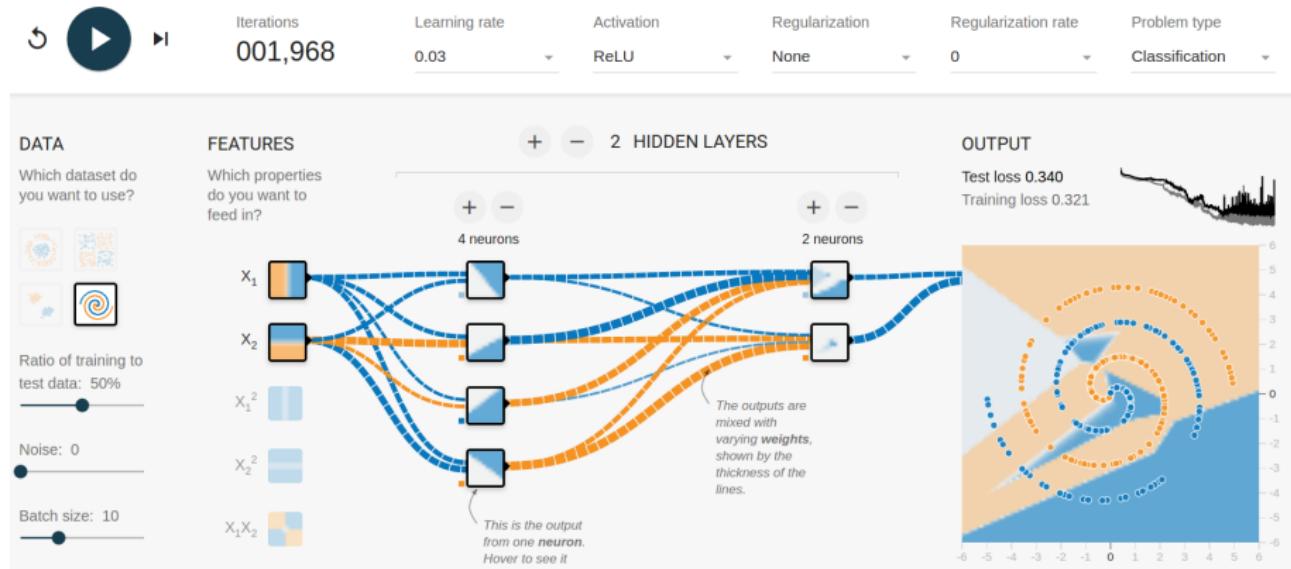
(<http://playground.tensorflow.org>)

Complex Target Function, Two Hidden Layers



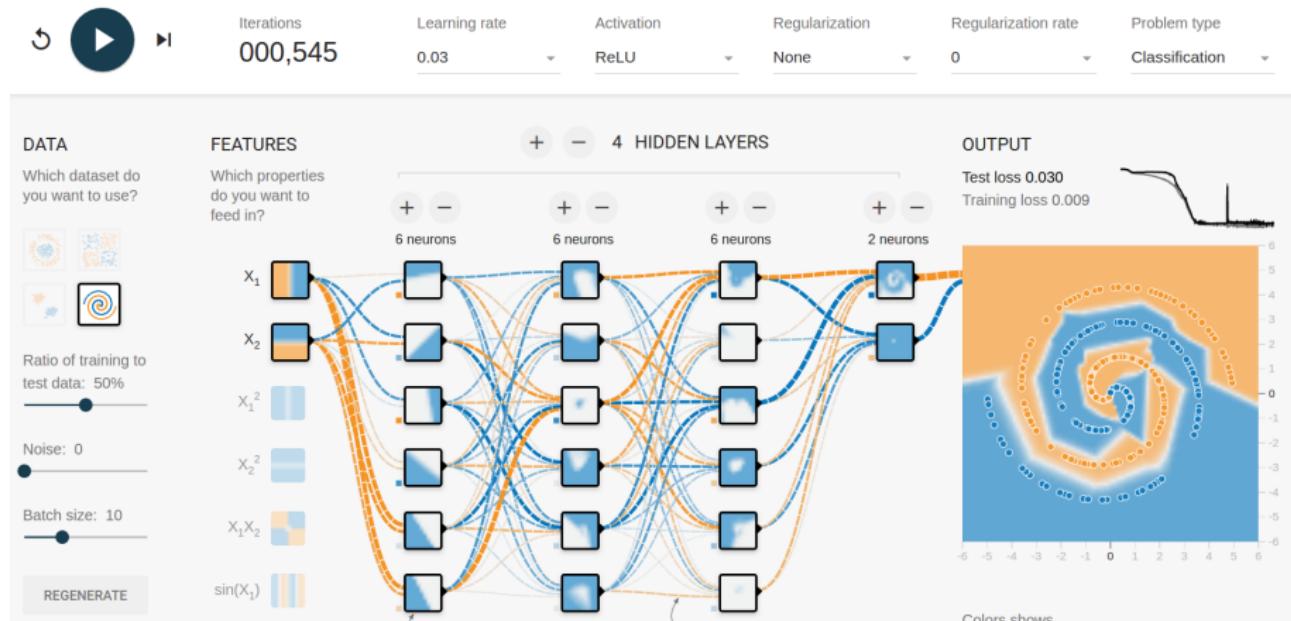
(<http://playground.tensorflow.org>)

Complex Target Function, Two Hidden Layers, ReLU



(<http://playground.tensorflow.org>)

Complex Target Function, Four Hidden Layers, ReLU



(<http://playground.tensorflow.org>)

Capacity of Neural Networks

Neural networks are excellent function approximators!

The universal approximation theorem is a nice result, but:

- We need a **learning algorithm** that finds the necessary parameter values
- ... and if we want to generalize, we need to control **overfitting**

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Training Neural Networks

We've seen that neural networks are very expressive—in theory, **they can approximate any function we want**

But to do so, their **parameters** $\theta := \{(\mathbf{W}^{(\ell)}, \mathbf{b}^{(\ell)})\}_{\ell=1}^{L+1}$ need to be set accordingly, for every layer

Key idea: **learn** these parameters from data

In other words: learn a function by sampling a few points and their values

(We've seen this already when we talked about linear models a few days ago...)

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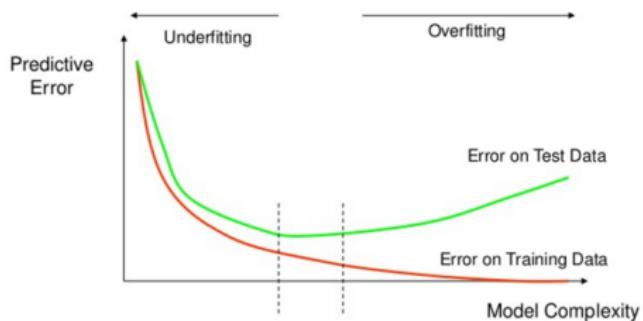
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Empirical Risk Minimization

Goal: choose parameters $\theta := \{(\mathbf{W}^{(\ell)}, \mathbf{b}^{(\ell)})\}_{\ell=1}^{L+1}$ that minimize the following objective function:

$$\mathcal{L}(\theta) := \lambda \Omega(\theta) + \frac{1}{N} \sum_{i=1}^N L(f(x_i; \theta), y_i)$$

- $\Omega(\theta)$ is a **regularizer**
- $L(f(x_i; \theta), y_i)$ is a **loss function**
- λ is a **regularization constant**
(an hyperparameter that needs to be tuned)



Recap: Gradient Descent

We can write the objective as:

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &:= \lambda\Omega(\boldsymbol{\theta}) + \frac{1}{N} \sum_{i=1}^N L(\mathbf{f}(\mathbf{x}_i; \boldsymbol{\theta}), y_i) \\ &:= \frac{1}{N} \sum_{i=1}^N \mathcal{L}_i(\boldsymbol{\theta}),\end{aligned}$$

where $\mathcal{L}_i = \lambda\Omega(\boldsymbol{\theta}) + L(\mathbf{f}(\mathbf{x}_i; \boldsymbol{\theta}), y_i)$

The gradient is:

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) := \frac{1}{N} \sum_{i=1}^N \nabla_{\boldsymbol{\theta}} \mathcal{L}_i(\boldsymbol{\theta})$$

Requires a full pass over the data before updating the weights—**too slow!**

Recap: Stochastic Gradient Descent

Key idea: sample a **single** training example uniformly (a random $j \in [N]$)

This way we get a noisy but **unbiased** estimate of the gradient:

$$\begin{aligned}\nabla_{\theta} \mathcal{L}(\theta) &:= \frac{1}{N} \sum_{i=1}^N \nabla_{\theta} \mathcal{L}_i(\theta) \\ &\approx \nabla_{\theta} \mathcal{L}_j(\theta) \\ &= \lambda \nabla_{\theta} \Omega(\theta) + \nabla_{\theta} L(f(x_j; \theta), y_j).\end{aligned}$$

The weights $\theta = \{(\mathbf{W}^{(\ell)}, \mathbf{b}^{(\ell)})\}_{\ell=1}^{L+1}$ are then updated as:

$$\theta \leftarrow \theta - \eta \nabla_{\theta} \mathcal{L}_j(\theta)$$

In practice, we often use a **mini-batch** instead of a single example!

Stochastic Gradient Descent with Mini-Batches

With a mini-batch $\{j_1, \dots, j_B\}$ ($B \ll N$) we get a less noisy, still **unbiased** estimate of the gradient:

$$\begin{aligned}\nabla_{\theta} \mathcal{L}(\theta) &:= \frac{1}{N} \sum_{i=1}^N \nabla_{\theta} \mathcal{L}_i(\theta) \\ &\approx \frac{1}{B} \sum_{i=1}^B \nabla_{\theta} \mathcal{L}_{j_i}(\theta) \\ &= \lambda \nabla_{\theta} \Omega(\theta) + \frac{1}{B} \sum_{i=1}^B \nabla_{\theta} L(f(x_{j_i}; \theta), y_{j_i}).\end{aligned}$$

The weights $\theta = \{(\mathbf{W}^{(\ell)}, \mathbf{b}^{(\ell)})\}_{\ell=1}^{L+1}$ are then updated as:

$$\theta \leftarrow \theta - \eta \frac{1}{B} \sum_{i=1}^B \nabla_{\theta} \mathcal{L}_{j_i}(\theta)$$

The Key Ingredients of SGD

In sum, we need the following ingredients:

- The loss function $L(f(x_i; \theta), y_i)$;
- A procedure for computing the gradients $\nabla_{\theta} L(f(x_i; \theta), y_i)$;
- The regularizer $\Omega(\theta)$ and its gradient.

Let's see them one at the time...

Loss Function

Should match as much as possible the metric we want to optimize at test time

Should be well-behaved (continuous, maybe smooth) to be amenable to optimization (this rules out the 0/1 loss)

Some examples:

- Squared loss for regression
- Negative log-likelihood (cross-entropy) for multi-class classification
- Sparsemax loss for multi-class and multi-label classification

Squared Loss

- The common choice for regression/reconstruction problems
- The neural network estimates $\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}) \approx \mathbf{y}$
- We minimize the **mean squared error**:

$$L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), \mathbf{y}) = \frac{1}{2} \|\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}) - \mathbf{y}\|^2$$

- Loss gradient:

$$\frac{\partial L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}, \mathbf{y}))}{\partial f_c(\mathbf{x}; \boldsymbol{\theta})} = f_c(\mathbf{x}; \boldsymbol{\theta}) - y_c$$

Negative Log-Likelihood (Cross-Entropy)

- The common choice for a softmax output layer
- The neural network estimates $f_c(x; \theta) \approx P(y = c | x)$
- We minimize the negative log-likelihood (also called **cross-entropy**):

$$\begin{aligned} L(\mathbf{f}(x; \theta), y) &= - \sum_c 1_{(y=c)} \log f_c(x; \theta) \\ &= - \log f_y(x; \theta) \\ &= - \log \text{softmax}(z(x)), \end{aligned}$$

where z is the **output pre-activation**.

- Loss gradient at output pre-activation:

$$\frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial z_c} = -(1_{(y=c)} - \text{softmax}_c(z(x)))$$

Sparsemax Loss (Martins and Astudillo, 2016)

- The natural choice for a sparsemax output layer
- The neural network estimates $f_c(x; \theta) \approx p(y = c | x)$ as a **sparse distribution**

$$L(\mathbf{f}(x; \theta), y) = -z_c + \frac{1}{2} \sum_{j \in S(z)} (z_j^2 - \tau^2(z)) + \frac{1}{2},$$

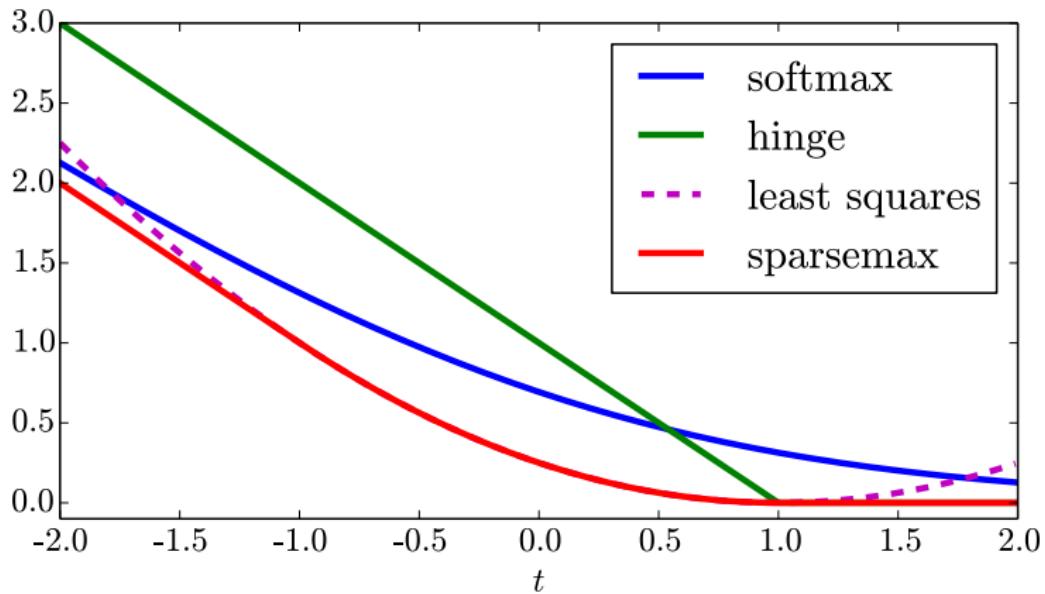
where z is the **output pre-activation**, $S(z)$ is the support of $p(y | x)$ and $\tau^2 : \mathbb{R}^K \rightarrow \mathbb{R}$ is the square of the threshold function (see Martins and Astudillo (2016) for details).

- Loss gradient at output pre-activation:

$$\frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial z_c} = -(1_{(y=c)} - \text{sparsemax}_c(z(x)))$$

Classification Losses in Two Dimensions

- Let the correct label be $y = 1$ and define $t = z_1 - z_2$:



The Key Ingredients of SGD

In sum, we need the following ingredients:

- The loss function $L(f(x_i; \theta), y_i)$;
- A procedure for computing the gradients $\nabla_{\theta} L(f(x_i; \theta), y_i)$ – **next!**
- The regularizer $\Omega(\theta)$ and its gradient.

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Gradient Computation

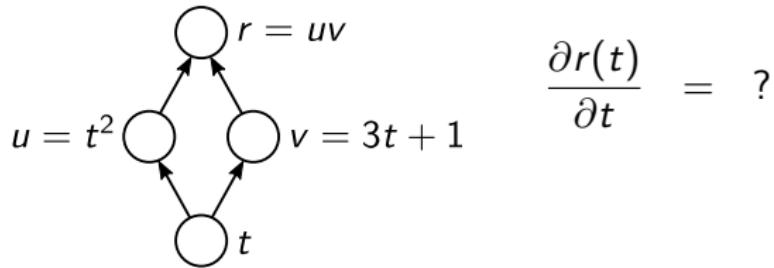
- Recall that we need to compute

$$\nabla_{\theta} L(f(x_i; \theta), y_i)$$

for $\theta = \{(\mathbf{W}^{(\ell)}, \mathbf{b}^{(\ell)})\}_{\ell=1}^{L+1}$ (the weights and biases at all layers)

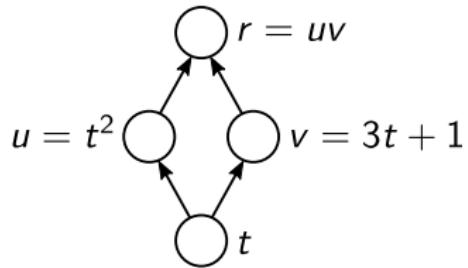
- This will be done with the **gradient backpropagation algorithm**
- **Key idea:** use the chain rule for derivatives!

Recap: Chain Rule



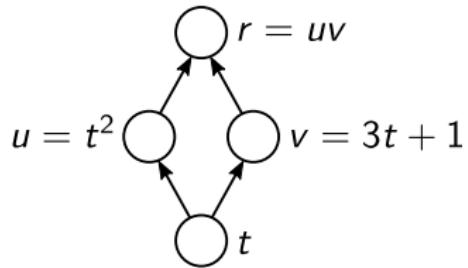
$$\frac{\partial r(t)}{\partial t} = ?$$

Recap: Chain Rule



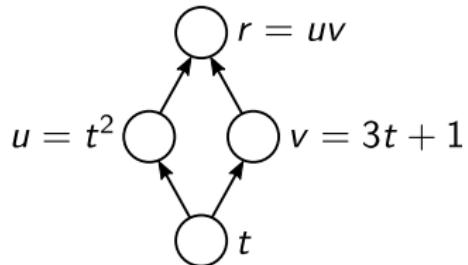
$$\frac{\partial r(t)}{\partial t} = \frac{\partial r(u)}{\partial u} \frac{\partial u(t)}{\partial t} + \frac{\partial r(v)}{\partial v} \frac{\partial v(t)}{\partial t}$$

Recap: Chain Rule



$$\begin{aligned}\frac{\partial r(t)}{\partial t} &= \frac{\partial r(u)}{\partial u} \frac{\partial u(t)}{\partial t} + \frac{\partial r(v)}{\partial v} \frac{\partial v(t)}{\partial t} \\ &= 2tv + 3u \\ &= 2t(3t + 1) + 3t^2 = 9t^2 + 2t.\end{aligned}$$

Recap: Chain Rule



$$\begin{aligned}\frac{\partial r(t)}{\partial t} &= \frac{\partial r(u)}{\partial u} \frac{\partial u(t)}{\partial t} + \frac{\partial r(v)}{\partial v} \frac{\partial v(t)}{\partial t} \\ &= 2tv + 3u \\ &= 2t(3t + 1) + 3t^2 = 9t^2 + 2t.\end{aligned}$$

- If a function $r(t)$ can be written as a function of intermediate results $q_i(t)$, then we have:

$$\frac{\partial r(t)}{\partial t} = \sum_i \frac{\partial r(t)}{\partial q_i(t)} \frac{\partial q_i(t)}{\partial t}$$

- We can invoke it by setting t to a output unit in a layer; $q_i(t)$ to the pre-activation in the layer above; and $r(t)$ to the loss function.

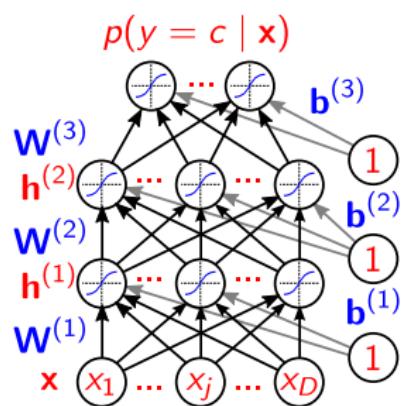
Hidden Layer Gradient

Main message: gradient backpropagation is just the chain rule of derivatives!

Hidden Layer Gradient

(Recap: $\mathbf{z}^{(\ell+1)} = \mathbf{W}^{(\ell+1)}\mathbf{h}^{(\ell)} + \mathbf{b}^{(\ell+1)}$)

$$\begin{aligned}\frac{\partial L(\mathbf{f}(\mathbf{x}; \theta), y)}{\partial h_j^{(\ell)}} &= \sum_i \frac{\partial L(\mathbf{f}(\mathbf{x}; \theta), y)}{\partial z_i^{(\ell+1)}} \frac{\partial z_i^{(\ell+1)}}{\partial h_j^{(\ell)}} \\ &= \sum_i \frac{\partial L(\mathbf{f}(\mathbf{x}; \theta), y)}{\partial z_i^{(\ell+1)}} \mathbf{W}_{i,j}^{(\ell+1)}\end{aligned}$$

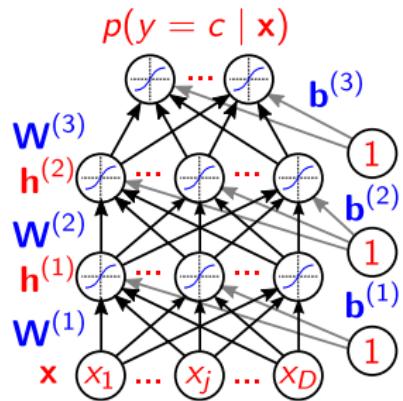


Hence $\nabla_{\mathbf{h}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) = \mathbf{W}^{(\ell+1)^\top} \nabla_{\mathbf{z}^{(\ell+1)}} L(\mathbf{f}(\mathbf{x}; \theta), y)$.

Hidden Layer Gradient (Before Activation)

(Recap: $h_j^{(\ell)} = g(z_j^{(\ell)})$, where $g : \mathbb{R} \rightarrow \mathbb{R}$ is the activation function)

$$\begin{aligned}\frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial z_j^{(\ell)}} &= \frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial h_j^{(\ell)}} \frac{\partial h_j^{(\ell)}}{\partial z_j^{(\ell)}} \\ &= \frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial h_j^{(\ell)}} g'(z_j^{(\ell)})\end{aligned}$$



Hence $\nabla_{z^{(\ell)}} L(\mathbf{f}(x; \theta), y) = \nabla_{h^{(\ell)}} L(\mathbf{f}(x; \theta), y) \odot g'(z^{(\ell)})$.

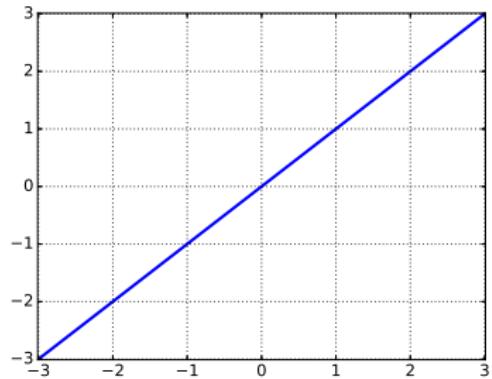
How to compute the derivative of the activation function $g'(z^{(\ell)})$?

Linear Activation

$$g(z) = z$$

Derivative:

$$g'(z) = 1$$

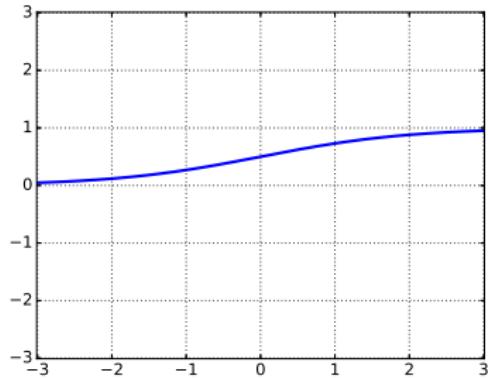


Sigmoid Activation

$$g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}$$

Derivative:

$$g'(z) = g(z)(1 - g(z))$$

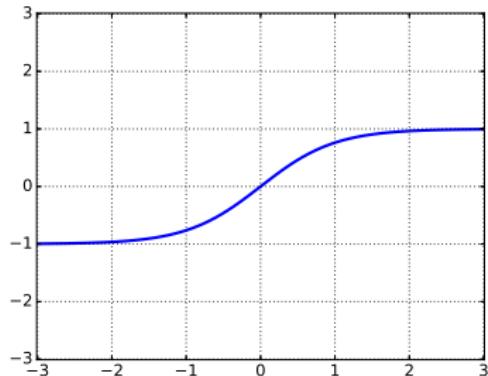


Hyperbolic Tangent Activation

$$g(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

Derivative:

$$g'(z) = 1 - g(z)^2$$

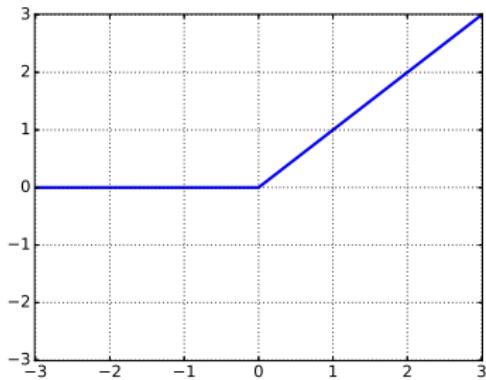


Rectified Linear Unit Activation (Glorot et al., 2011)

$$g(z) = \text{relu}(z) = \max\{0, z\}$$

Derivative (except for $z = 0$):

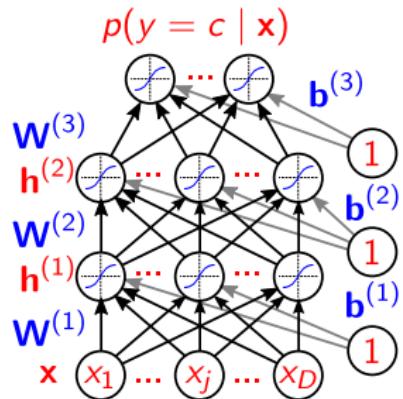
$$g'(z) = 1_{z>0}$$



Parameter Gradient

(Recap: $z^{(\ell)} = \mathbf{W}^{(\ell)} \mathbf{h}^{(\ell-1)} + \mathbf{b}^{(\ell)}$)

$$\begin{aligned}\frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial \mathbf{W}_{i,j}^{(\ell)}} &= \frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial z_i^{(\ell)}} \frac{\partial z_i^{(\ell)}}{\partial \mathbf{W}_{i,j}^{(\ell)}} \\ &= \frac{\partial L(\mathbf{f}(x; \theta), y)}{\partial z_i^{(\ell)}} h_j^{(\ell-1)}\end{aligned}$$



Hence $\nabla_{\mathbf{W}^{(\ell)}} L(\mathbf{f}(x; \theta), y) = \nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(x; \theta), y) \mathbf{h}^{(\ell-1)^\top}$

Similarly, $\nabla_{\mathbf{b}^{(\ell)}} L(\mathbf{f}(x; \theta), y) = \nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(x; \theta), y)$

Backpropagation

Compute output gradient (before activation):

$$\nabla_{\mathbf{z}^{(L+1)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) = -(\mathbf{1}_y - \mathbf{f}(\mathbf{x}))$$

for ℓ from $L + 1$ to 1 **do**

 Compute gradients of hidden layer parameters:

$$\nabla_{\mathbf{W}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) = \nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) \mathbf{h}^{(\ell-1)^\top}$$

$$\nabla_{\mathbf{b}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) = \nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y)$$

 Compute gradient of hidden layer below:

$$\nabla_{\mathbf{h}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) = \mathbf{W}^{(\ell+1)^\top} \nabla_{\mathbf{z}^{(\ell+1)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y)$$

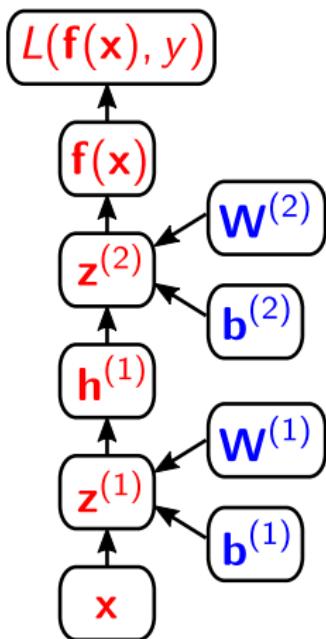
 Compute gradient of hidden layer below (before activation):

$$\nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) = \nabla_{\mathbf{h}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), y) \odot \mathbf{g}'(\mathbf{z}^{(\ell)})$$

end for

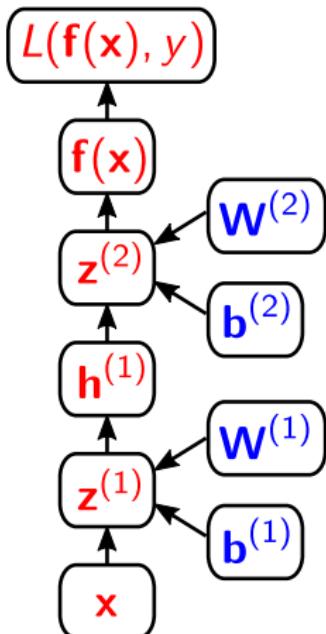
Computation Graph

- Forward propagation can be represented as a DAG
- Allows to implement forward propagation in a modular way
- Each box can be an object with a `fprop` method, that computes the value of the box given its children
- Calling the `fprop` method of each box in the right order (after a topological sort) yields forward propagation



Automatic Differentiation

- ... Also allows to implement backpropagation in a modular way
- Each box can also have a `bprop` method, that computes the loss gradient with respect to its children, given the loss gradient with respect to the output
- Can make use of cached computation done during the `fprop` method
- By calling the `bprop` method in reverse order, we get backpropagation (only need to reach the parameters)



Several Autodiff Strategies

Symbol-to-number differentiation (Caffe, Torch, Pytorch, Dynet, ...)

- Take a computational graph and a set of numerical inputs, then return a set of numerical values describing the gradient at those input values
- Advantage: simpler to implement and to debug
- Disadvantage: only works for first-order derivatives

Symbol-to-symbol differentiation (Theano, Tensorflow, ...)

- Take a computational graph and add additional nodes to the graph that provide a symbolic description of the desired derivatives (i.e. the derivatives are just another computational graph)
- Advantage: generalizes automatically to higher-order derivatives
- Disadvantage: harder to implement and to debug

Many Software Toolkits for Neural Networks

- Theano
- Tensorflow
- Torch, Pytorch
- MXNet
- Keras
- Caffe
- DyNet
- ...



All implement automatic differentiation.

We will have a Pytorch tutorial next class (TA guest lecture)
Please bring your laptops!

Some Theano Code (Logistic Regression)

```
import numpy
import theano
import theano.tensor as T
rng = numpy.random

N = 400                      # training sample size
feats = 784                    # number of input variables

# generate a dataset: D = (input_values, target_class)
D = (rng.randn(N, feats), rng.randint(size=N, low=0, high=2))
training_steps = 10000

# Declare Theano symbolic variables
x = T.dmatrix("x")
y = T.dvector("y")

# initialize the weight vector w randomly
#
# this and the following bias variable b
# are shared so they keep their values
# between training iterations (updates)
w = theano.shared(rng.randn(feats), name="w")

# initialize the bias term
b = theano.shared(0., name="b")

print("Initial model:")
print(w.get_value())
print(b.get_value())

# Construct Theano expression graph
p_1 = 1 / (1 + T.exp(-T.dot(x, w) - b))    # Probability that target = 1
prediction = p_1 > 0.5                         # The prediction thresholded
xent = -y * T.log(p_1) - (1-y) * T.log(1-p_1) # Cross-entropy loss function
cost = xent.mean() + 0.01 * (w ** 2).sum()       # The cost to minimize
gw, gb = T.grad(cost, [w, b])                   # Compute the gradient of the cost
                                                # w.r.t weight vector w and
                                                # bias term b
                                                # (we shall return to this in a
                                                # following section of this tutorial)

# Compile
train = theano.function([x, y], [prediction, cost],
                        givens={w: gw, b: gb},
                        on_unused_input='ignore')
```

Some Code in Tensorflow (Linear Regression)

```
import tensorflow as tf
import numpy as np

# Create 100 phony x, y data points in NumPy, y = x * 0.1 + 0.3
x_data = np.random.rand(100).astype(np.float32)
y_data = x_data * 0.1 + 0.3

# Try to find values for W and b that compute y_data = W * x_data + b
# (We know that W should be 0.1 and b 0.3, but TensorFlow will
# figure that out for us.)
W = tf.Variable(tf.random_uniform([1], -1.0, 1.0))
b = tf.Variable(tf.zeros([1]))
y = W * x_data + b

# Minimize the mean squared errors.
loss = tf.reduce_mean(tf.square(y - y_data))
optimizer = tf.train.GradientDescentOptimizer(0.5)
train = optimizer.minimize(loss)

# Before starting, initialize the variables. We will 'run' this first.
init = tf.global_variables_initializer()

# Launch the graph.
sess = tf.Session()
sess.run(init)

# Fit the line.
for step in range(201):
    sess.run(train)
    if step % 20 == 0:
        print(step, sess.run(W), sess.run(b))

# Learns best fit is W: [0.1], b: [0.3]
```

Some Code in Keras (Multi-Layer Perceptron)

Multilayer Perceptron (MLP) for multi-class softmax classification:

```
from keras.models import Sequential
from keras.layers import Dense, Dropout, Activation
from keras.optimizers import SGD

model = Sequential()
# Dense(64) is a fully-connected layer with 64 hidden units.
# in the first layer, you must specify the expected input data shape:
# here, 20-dimensional vectors.
model.add(Dense(64, input_dim=20, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(64, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(10, init='uniform'))
model.add(Activation('softmax'))

sgd = SGD(lr=0.1, decay=1e-6, momentum=0.9, nesterov=True)
model.compile(loss='categorical_crossentropy',
              optimizer=sgd,
              metrics=['accuracy'])

model.fit(X_train, y_train,
          nb_epoch=20,
          batch_size=16)
score = model.evaluate(X_test, y_test, batch_size=16)
```

Reminder: The Key Ingredients of SGD

In sum, we need the following ingredients:

- The loss function $L(f(x_i; \theta), y_i)$;
- A procedure for computing the gradients $\nabla_{\theta} L(f(x_i; \theta), y_i)$
- The regularizer $\Omega(\theta)$ and its gradient – **next!**

Regularization

Recall that we're minimizing the following objective function:

$$\mathcal{L}(\boldsymbol{\theta}) := \lambda \Omega(\boldsymbol{\theta}) + \frac{1}{N} \sum_{n=1}^N L(\mathbf{f}(\mathbf{x}_i; \boldsymbol{\theta}), y_i)$$

It remains to define the **regularizer** and its gradient

We'll talk about:

- ℓ_2 regularization
- ℓ_1 regularization
- dropout regularization

ℓ_2 Regularization

- Gaussian prior on the weights
- Note: only the weights are regularized (not the biases)

$$\Omega(\boldsymbol{\theta}) = \frac{1}{2} \sum_{\ell} \|\mathbf{W}^{(\ell)}\|^2$$

- Gradient is:

$$\nabla_{\mathbf{W}^{(\ell)}} \Omega(\boldsymbol{\theta}) = \mathbf{W}^{(\ell)}$$

- This has the effect of a weight decay:

$$\begin{aligned}\mathbf{W}^{(\ell)} &\leftarrow \mathbf{W}^{(\ell)} - \eta \nabla_{\mathbf{W}^{(\ell)}} \mathcal{L}_i(\boldsymbol{\theta}) \\&= \mathbf{W}^{(\ell)} - \eta (\lambda \nabla_{\mathbf{W}^{(\ell)}} \Omega(\boldsymbol{\theta}) + \nabla_{\mathbf{W}^{(\ell)}} L(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i)) \\&= (1 - \eta \lambda) \mathbf{W}^{(\ell)} - \eta \nabla_{\mathbf{W}^{(\ell)}} L(f(\mathbf{x}_i; \boldsymbol{\theta}), y_i)\end{aligned}$$

ℓ_1 Regularization

- Laplacian prior on the weights
- Note: only the weights are regularized (not the biases)

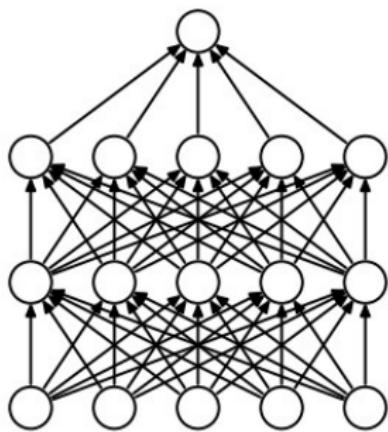
$$\Omega(\theta) = \sum_{\ell} \|\mathbf{W}^{(\ell)}\|_1$$

- Gradient is:

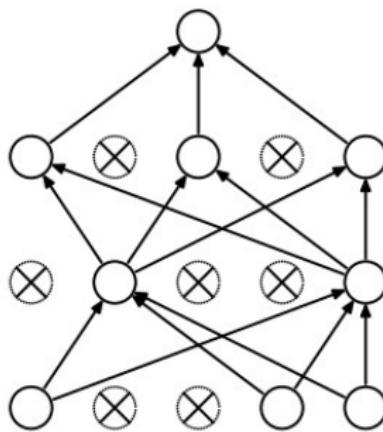
$$\nabla_{\mathbf{W}^{(\ell)}} \Omega(\theta) = \mathbf{sign}(\mathbf{W}^{(\ell)})$$

- Promotes sparsity of the weights

Dropout Regularization (Srivastava et al., 2014)



(a) Standard Neural Net



(b) After applying dropout.

Idea: During training, remove some hidden units stochastically

Dropout Regularization (Srivastava et al., 2014)

- Each hidden unit's output is set to 0 with probability p (e.g. $p = 0.5$)
- This prevents hidden units to co-adapt to other units, forcing them to be more generally useful
- At test time, keep all units, but multiply their outputs by $1 - p$
- Shown to be a form of adaptive regularization (Wager et al., 2013)
- Note: many software packages implement another variant, **inverted dropout**, where at training time the output of the units that were not dropped is divided by $1 - p$ and requires no change at test time

Implementation of Dropout

- This is usually implemented using random binary masks
- The hidden layer activations become (for $\ell = 1, \dots, L$):

$$h^{(\ell)}(x) = g(z^{(\ell)}(x)) \odot m^{(\ell)}$$

- Beats regular backpropagation on many datasets (Hinton et al., 2012)
- Other variants, e.g. DropConnect (Wan et al., 2013), Stochastic Pooling (Zeiler and Fergus, 2013)

Backpropagation with Dropout

Compute output gradient (before activation):

$$\nabla_{\mathbf{z}^{(L+1)}} L(\mathbf{f}(\mathbf{x}; \theta), y) = -(\mathbf{1}_y - \mathbf{f}(\mathbf{x}))$$

for ℓ from $L + 1$ to 1 **do**

Compute gradients of hidden layer parameters:

$$\nabla_{\mathbf{W}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) = \nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) \underbrace{\mathbf{h}^{(\ell-1)^\top}}_{\text{includes } \mathbf{m}^{(\ell-1)}}$$

$$\nabla_{\mathbf{b}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) = \nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y)$$

Compute gradient of hidden layer below:

$$\nabla_{\mathbf{h}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) = \mathbf{W}^{(\ell+1)^\top} \nabla_{\mathbf{z}^{(\ell+1)}} L(\mathbf{f}(\mathbf{x}; \theta), y)$$

Compute gradient of hidden layer below (before activation):

$$\nabla_{\mathbf{z}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) = \nabla_{\mathbf{h}^{(\ell)}} L(\mathbf{f}(\mathbf{x}; \theta), y) \odot \mathbf{g}'(\mathbf{z}^{(\ell)}) \odot \mathbf{m}^{(\ell-1)}$$

end for

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Initialization

Initialize all biases to zero

For weights:

- Cannot initialize to zero with **tanh** activation (the gradients would also be zero and we would reach a saddle point)
- Cannot initialize the weights to the same value (need to break the symmetry)
- Random initialization (Gaussian, uniform), sampling around 0 to break symmetry
- For ReLU activations, the mean should be a small positive number
- Variance cannot be too high, otherwise all neuron activations will be saturated

“Glorot Initialization”

- Recipe from Glorot and Bengio (2010):

$$\mathbf{W}_{i,j}^{(\ell)} \sim U[-t, t], \text{ with } t = \frac{\sqrt{6}}{\sqrt{K^{(\ell)} + K^{(\ell-1)}}}$$

- Works well in practice with **tanh** and sigmoid activations

Training, Validation, and Test Sets

Split datasets in training, validation, and test partitions.

- Training set serves to train the model
- Validation set serves to tune hyperparameters (learning rate, number of hidden units, regularization coefficient, dropout probability, best epoch, etc.)
- Test set serves to estimate the generalization performance

Hyperparameter Tuning: Grid Search, Random Search

Search for the best configuration of the hyperparameters:

- Grid search: specify a set of values we want to test for each hyperparameter, and try all configurations of these values
- Random search: specify a distribution over the values of each hyper-parameter (e.g. uniform in some range) and sample independently each hyper-parameter to get configurations
- Bayesian optimization and learning to learn (Snoek et al., 2012)

We can always go back and fine-tune the grid/distributions if necessary

Early Stopping

- To select the number of epochs, stop training when validation error increases (with some look ahead)
- One common strategy (with SGD) is to halve the learning rate for every epoch where the validation error increases



(Image credit: Hugo Larochelle)

Tricks of the Trade

- Normalization of the data
- Decaying the learning rate
- Mini-batches
- Adaptive learning rates
- Gradient checking
- Debugging on a small dataset

Normalization of the Data

- For each input dimension: subtract the training set mean and divide by the training set standard deviation
- This makes each input dimension have zero mean, unit variance
- This can speed up training (in number of epochs)
- Doesn't work for sparse inputs (destroys sparsity)

Decaying the Learning Rate

In SGD, as we get closer to a local minimum, it makes sense to take smaller update steps (to avoid diverging)

- Start with a large learning rate (say 0.1)
- Keep it fixed while validation error keeps improving
- Divide by 2 and go back to the previous step

Mini-Batches

- Instead of updating after a single example, can aggregate a mini-batch of examples (e.g. 50–200 examples) and compute the averaged gradient for the entire mini-batch
- Less noisy than vanilla SGD
- Can leverage matrix-matrix computations (or tensor computations)
- Large computational speed-ups in GPUs (since computation is trivially parallelizable across the mini-batch and we can exhaust the GPU memory)

Adaptive Learning Rates

Instead of using the same step size for all parameters, have one learning rate per parameter

- **Adagrad** (Duchi et al., 2011): learning rates are scaled by the square root of the cumulative sum of squared gradients

$$\eta^{(t)} = \eta^{(t-1)} + (\nabla_{\theta} L(\mathbf{f}(\mathbf{x}), y))^2, \quad \bar{\nabla}_{\theta}^{(t)} = \frac{\nabla_{\theta} L(\mathbf{f}(\mathbf{x}), y)}{\sqrt{\eta^{(t)} + \epsilon}}$$

- **RMSprop** (Tieleman and Hinton, 2012): instead of cumulative sum, use exponential moving average

$$\eta^{(t)} = \beta \eta^{(t-1)} + (1 - \beta)(\nabla_{\theta} L(\mathbf{f}(\mathbf{x}), y))^2, \quad \bar{\nabla}_{\theta}^{(t)} = \frac{\nabla_{\theta} L(\mathbf{f}(\mathbf{x}), y)}{\sqrt{\eta^{(t)} + \epsilon}}$$

- **Adam** (Kingma and Ba, 2014): combine RMSProp with momentum

Gradient Checking

- If the training loss is not decreasing even with a very small learning rate, there's likely a bug in the gradient computation
- To debug your implementation of fprop/bprop, compute the “numeric gradient,” a finite difference approximation of the true gradient:

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x + \epsilon) - f(x - \epsilon)}{2\epsilon}$$

Debugging on a Small Dataset

- Extract a small subset of your training set (e.g. 50 examples)
- Monitor your training loss in this set
- You should be able to overfit in this small training set
- If not, see if some units are saturated from the very first iterations (if they are, reduce the initialization variance or properly normalize your inputs)
- If the training error is bouncing up and down, decrease the learning rate

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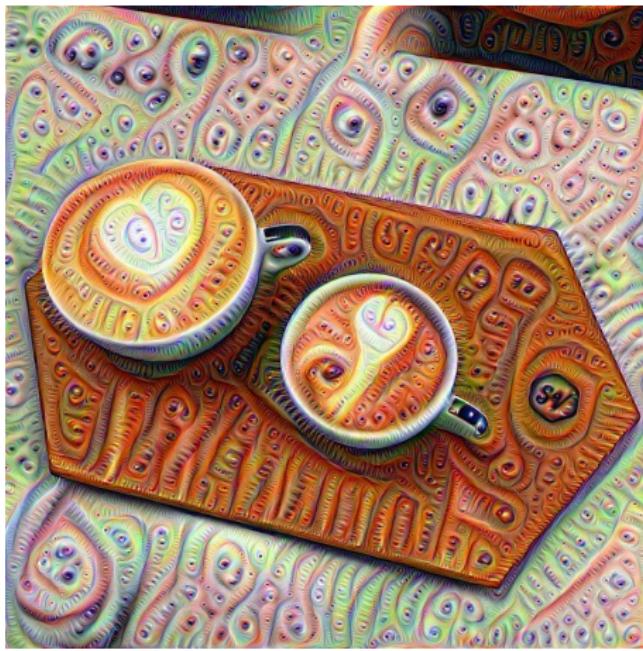
③ Conclusions

Conclusions

- Multi-layer perceptrons are universal function approximators
- However, they need to be trained
- Stochastic gradient descent is an effective training algorithm
- This is possible with the gradient backpropagation algorithm (an application of the chain rule of derivatives)
- Most current software packages represent a computation graph and implement automatic differentiation
- Dropout regularization is effective to avoid overfitting

Thank you!

Questions?



References I

- Cybenko, G. (1989). Approximation by superpositions of a sigmoidal function. *Mathematics of control, signals and systems*, 2(4):303–314.
- Duchi, J., Hazan, E., and Singer, Y. (2011). Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, 12(Jul):2121–2159.
- Glorot, X. and Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. In *AISTATS*, volume 9, pages 249–256.
- Glorot, X., Bordes, A., and Bengio, Y. (2011). Deep Sparse Rectifier Neural Networks. In *International Conference on Artificial Intelligence and Statistics*, pages 315–323.
- Hinton, G. E., Srivastava, N., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. R. (2012). Improving neural networks by preventing co-adaptation of feature detectors. *arXiv preprint arXiv:1207.0580*.
- Hornik, K., Stinchcombe, M., and White, H. (1989). Multilayer feedforward networks are universal approximators. *Neural networks*, 2(5):359–366.
- Kingma, D. and Ba, J. (2014). Adam: A Method for Stochastic Optimization. In *Proc. of International Conference on Learning Representations*.
- Martins, A. F. T. and Astudillo, R. (2016). From Softmax to Sparsemax: A Sparse Model of Attention and Multi-Label Classification. In *Proc. of the International Conference on Machine Learning*.
- McCulloch, W. S. and Pitts, W. (1943). A logical calculus of the ideas immanent in nervous activity. *The bulletin of mathematical biophysics*, 5(4):115–133.
- Minsky, M. and Papert, S. (1969). Perceptrons.
- Montufar, G. F., Pascanu, R., Cho, K., and Bengio, Y. (2014). On the number of linear regions of deep neural networks. In *Advances in Neural Information Processing Systems*, pages 2924–2932.
- Snoek, J., Larochelle, H., and Adams, R. P. (2012). Practical bayesian optimization of machine learning algorithms. In *Advances in neural information processing systems*, pages 2951–2959.
- Srivastava, N., Hinton, G. E., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. *Journal of Machine Learning Research*, 15(1):1929–1958.

References II

- Tieleman, T. and Hinton, G. (2012). Rmsprop: Divide the gradient by a running average of its recent magnitude. *COURSERA: Neural Networks for Machine Learning*, 4(2).
- Wager, S., Wang, S., and Liang, P. S. (2013). Dropout training as adaptive regularization. In *Advances in neural information processing systems*, pages 351–359.
- Wan, L., Zeiler, M., Zhang, S., Cun, Y. L., and Fergus, R. (2013). Regularization of neural networks using dropconnect. In *Proc. of the International Conference on Machine Learning*, pages 1058–1066.
- Zeiler, M. D. and Fergus, R. (2013). Stochastic pooling for regularization of deep convolutional neural networks. *arXiv preprint arXiv:1301.3557*.