Lecture 3: Neural Networks

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Deep Structured Learning Course, Fall 2020

Announcements

Homework 1 is out! Deadline is October 28. Start early!!!

Deadline for project proposal: October 21 (two weeks from now)

- Check the course webpage for a list of project ideas!
- You need to turn in a 1-page proposal (NeurIPS format) explaining:
  - The type of project: survey or practical
  - The problem you propose to solve / the topic you will address
  - For surveys: motivation and list of main papers you will cover
  - For practical projects:
    - Which method(s) you are going to use
    - Which evaluation metric and which data you are going to use
- Team size: 3–4 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 funcions: 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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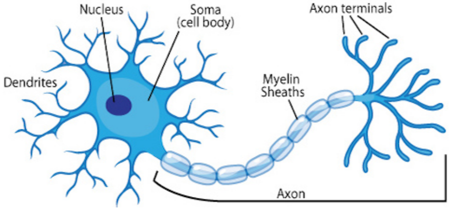
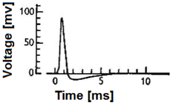
Biological Neuron

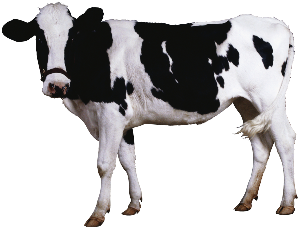




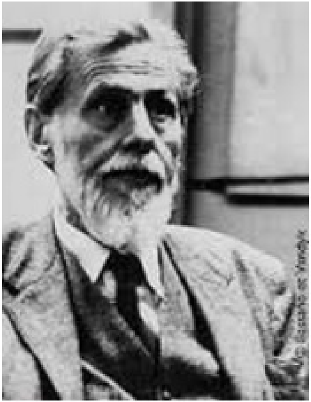
- Three main parts: the main body (soma), dendrites and an axon
- The neuron receives input signals from dendrites, and then outputs its own signals through the axon
- Axons in turn connect to the dendrites of other neurons, using special connections called synapses
- Generate sharp electrical potentials 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)

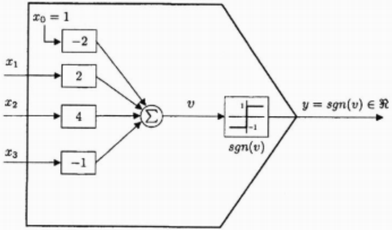
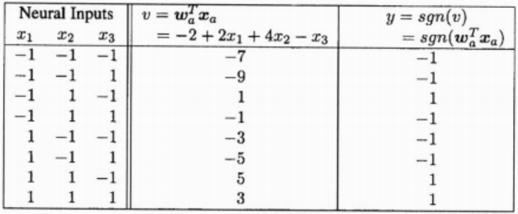


Figure 3.6 Example 3.2: a threshold neural logic for $y = x_2(x_1 + \overline{x}_3)$.

Table 3.6 **Truth table for Example 3.2**



Neural Inputs			$v = \boldsymbol{w}_a^T \boldsymbol{x}_a$	$y = sgn(v)$
x_1	x_2	x_3	$= -2 + 2x_1 + 4x_2 - x_3$	$= sgn(\boldsymbol{w}_a^T \boldsymbol{x}_a)$
-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

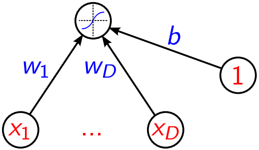
- Later models replaced the hard threshold by more general activations

Artificial Neuron

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

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

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



- **Activation:**

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

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

Outline

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   - Definition
   - Activations
   - Feed-forward Neural Networks
   - Universal Approximation
2. **Training Neural Networks**
   - Empirical Risk Minimization
   - Gradient Backpropagation
   - Tricks of the Trade
3. **Conclusions**

Activation Function

Typical choices:

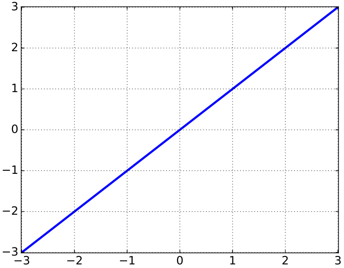
- Linear
- Sigmoid (logistic function)
- Hyperbolic Tangent
- Rectified Linear

Later:

- Softmax
- Sparsemax
- Max-pooling

Linear Activation

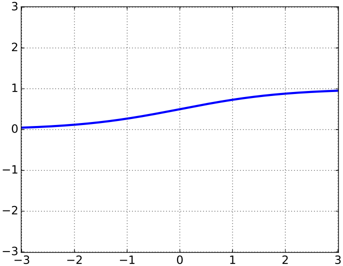
$$\boxed{g(z) = z}$$



- 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

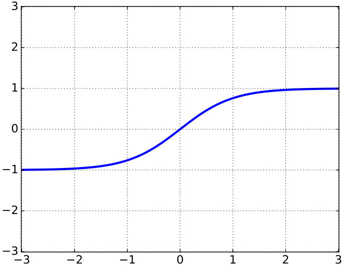
$$\boxed{g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}}$$



- "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

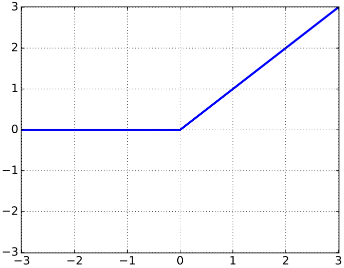
$$\boxed{g(z) = \mathbf{tanh}(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}}$$



- "Squashes" the neuron pre-activation between -1 and 1
- Related to the sigmoid via $\sigma(z) = \frac{1+\mathbf{tanh}(z/2)}{2}$
- 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)

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



- 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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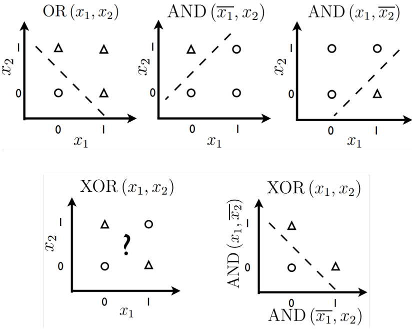
3. **Conclusions**

Capacity of Single Neuron (Linear Classifier)

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

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

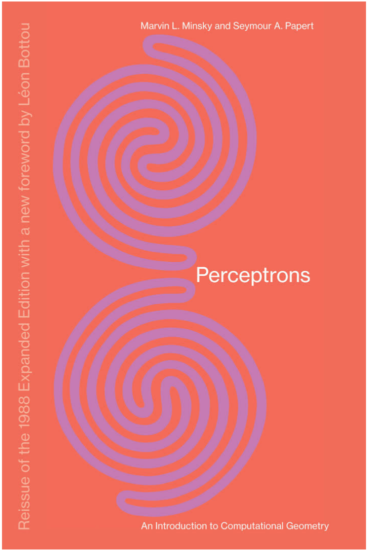
- Can solve linearly separable problems (OR, AND)
- Can't solve non-linearly separable problems (XOR)—unless input is transformed into a better representation



OR (x_1, x_2)
AND $(\overline{x_1}, x_2)$
AND $(x_1, \overline{x_2})$
x_1
x_2
0
1
XOR (x_1, x_2)
?
AND $(x_1, \overline{x_2})$
AND $(\overline{x_1}, x_2)$

(Slide credit: Hugo Larochelle)

The XOR Affair


Marvin L. Minsky and Seymour A. Papert
Perceptrons
An Introduction to Computational Geometry
Reissue of the 1988 Expanded Edition with a new foreword by Léon Bottou

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

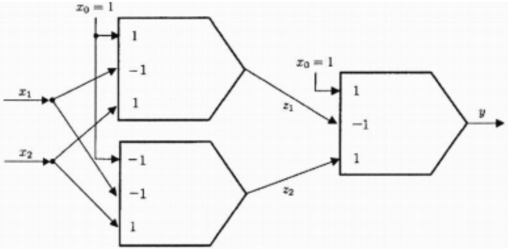


Figure 3.11 Example 3.6: a threshold network for *XOR* function $y = x_1 \oplus x_2 = sgn(1 - z_1 + z_2)$, $z_1 = sgn(1 - x_1 + x_2)$, $z_2 = sgn(-1 - x_1 + x_2)$.

Solving XOR with Multi-Layer Perceptron

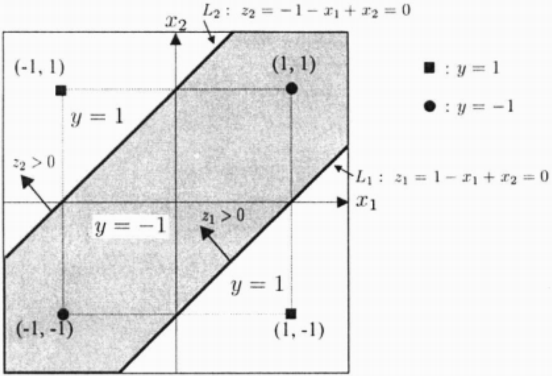


Figure 3.12 Example 3.6: two discriminant lines for *XOR* function $y = x_1 \oplus x_2$.

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

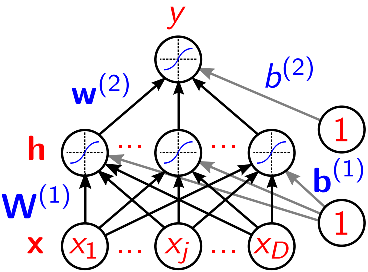
Multi-Layer Neural Network

- **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 ($\boldsymbol{x} \in \mathbb{R}^D$) but a single output (e.g. $y \in \mathbb{R}$ or $y \in \{0, 1\}$)

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



Single Hidden Layer

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

- **Hidden layer pre-activation:**

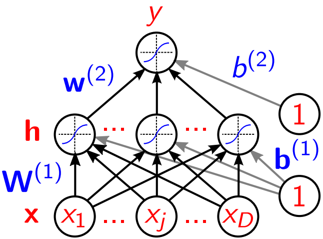
$$\boldsymbol{z}(\boldsymbol{x}) = \boldsymbol{W}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)},$$

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

- **Hidden layer activation:**

$$\boldsymbol{h}(\boldsymbol{z}) = \boldsymbol{g}(\boldsymbol{z}(\boldsymbol{x})),$$

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



- **Output layer activation:**

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

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

Single Hidden Layer

Overall,

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

Examples:

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

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

$\boldsymbol{h}$ 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 $p(y = c \mid \boldsymbol{x})$

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** : $\mathbb{R}^C \to \Delta^{C-1}$:

$$\boxed{\boldsymbol{o}(\boldsymbol{z}) = \textbf{softmax}(\boldsymbol{z}) = \left[\frac{\exp(z_1)}{\sum_c \exp(z_c)}, \ldots, \frac{\exp(z_C)}{\sum_c \exp(z_c)}\right]}$$

- We saw this already in class, when talking about logistic regression!
- Strictly positive, sums to 1
- Resulting distribution has full support: $\textbf{softmax}(\boldsymbol{z}) > \mathbf{0}, \forall \boldsymbol{z}$
- 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:

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

- In words: Euclidean projection of $\boldsymbol{z}$ onto the probability simplex
- Likely to hit the boundary of the simplex, in which case **sparsemax**($\boldsymbol{z}$) 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:

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

  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:** $\boldsymbol{z} \in \mathbb{R}^C$
Sort $\boldsymbol{z}$ as $z_{(1)} \geq \ldots \geq z_{(C)}$
Find $k(\boldsymbol{z}) := \max \left\{ k \in [C] \mid 1 + k z_{(k)} > \sum_{j \leq k} z_{(j)} \right\}$
Define $\tau(\boldsymbol{z}) = \frac{\left(\sum_{j \leq k(\boldsymbol{z})} z_{(j)}\right) - 1}{k(\boldsymbol{z})}$
**Output:** $\boldsymbol{p} \in \Delta^{C-1}$ s.t. $p_i = [z_i - \tau(\boldsymbol{z})]_+$.
```

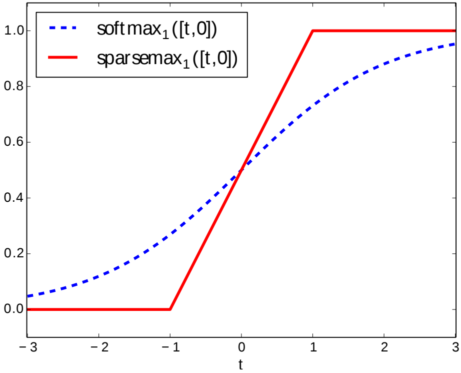
- Time complexity is $O(C \log C)$ due to the sort operation; but $O(C)$ algorithms exist based on linear-time selection.
- Note: evaluating **softmax** costs $\mathrm{O}(C)$ too.

Two Dimensions

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

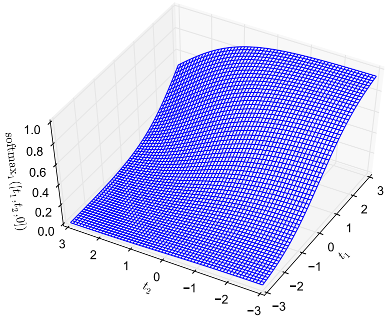
$$\textbf{softmax}_1(z) = (1 + \exp(-t))^{-1}$$

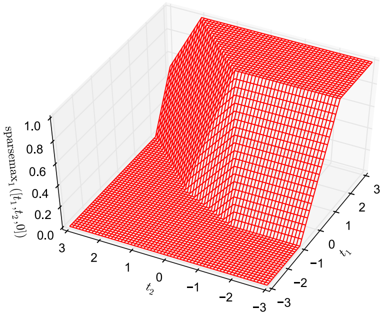
- The 2D **sparsemax** is the "hard" version of the sigmoid:



Three Dimensions

- Parameterize $\boldsymbol{z} = (t_1, t_2, 0)$ and plot $\textbf{softmax}_1(\boldsymbol{z})$ and $\textbf{sparsemax}_1(\boldsymbol{z})$ 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:

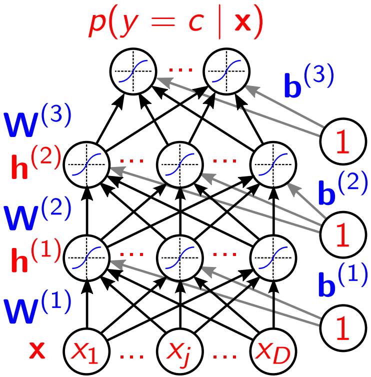
- **Hidden layer pre-activation** (define $\boldsymbol{h}^{(0)} = \boldsymbol{x}$ for convenience):

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

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

- **Hidden layer activation:**

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



- **Output layer activation:**

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

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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

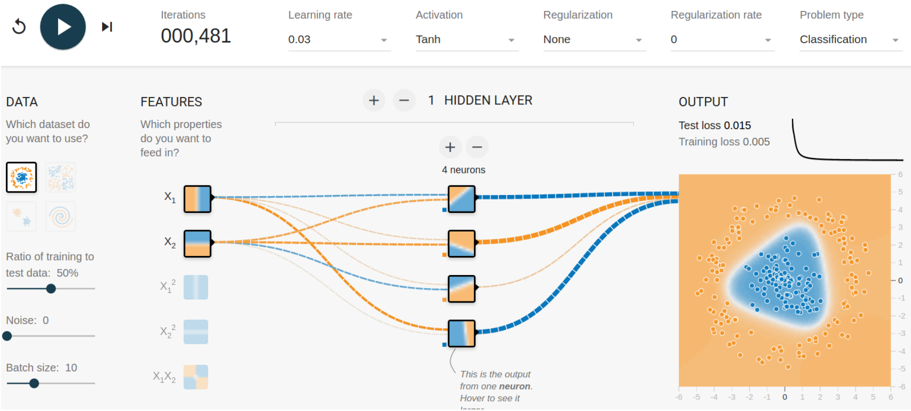
Theorem (Montufar et al. (2014))

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

$$O\left(\left(\begin{array}{c} K \\ D \end{array}\right)^{D(L-1)} K^D\right)$$

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

"Simple" Target Function, One Hidden Layer



Iterations 000,481

Learning rate 0.03

Activation Tanh

Regularization None

Regularization rate 0

Problem type Classification

DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

FEATURES

Which properties do you want to feed in?

1 HIDDEN LAYER

4 neurons

OUTPUT

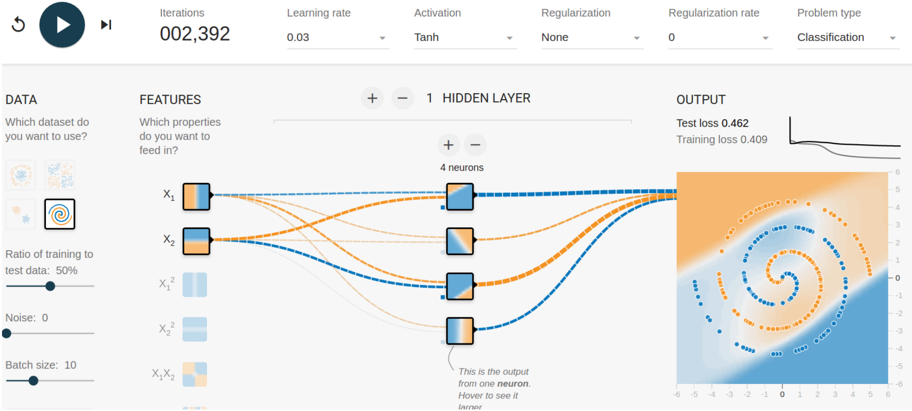
Test loss 0.015

Training loss 0.005

*This is the output from one **neuron**. Hover to see it larger.*

(http://playground.tensorflow.org)

Complex Target Function, One Hidden Layer



Iterations 002,392

Learning rate 0.03

Activation Tanh

Regularization None

Regularization rate 0

Problem type Classification

DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

FEATURES

Which properties do you want to feed in?

1 HIDDEN LAYER

4 neurons

*This is the output from one **neuron**. Hover to see it larger*

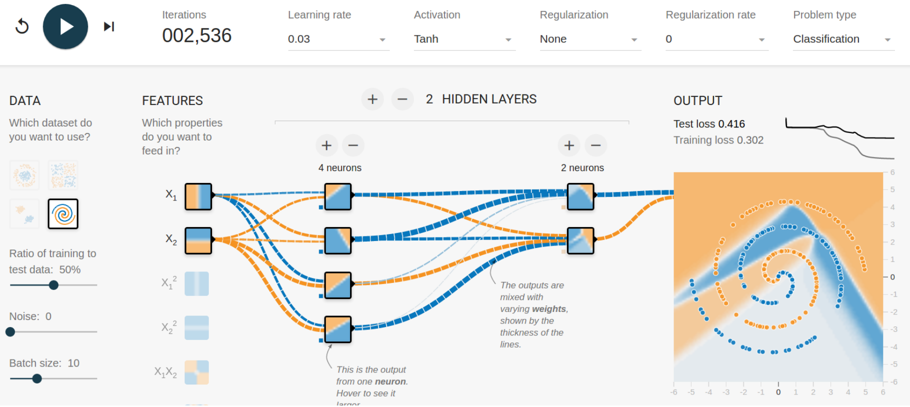
OUTPUT

Test loss 0.462

Training loss 0.409

(http://playground.tensorflow.org)

Complex Target Function, Two Hidden Layers



Iterations 002,536

Learning rate 0.03

Activation Tanh

Regularization None

Regularization rate 0

Problem type Classification

DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

FEATURES

Which properties do you want to feed in?

2 HIDDEN LAYERS

4 neurons

2 neurons

The outputs are mixed with varying **weights**, shown by the thickness of the lines.

This is the output from one **neuron**. Hover to see it larger

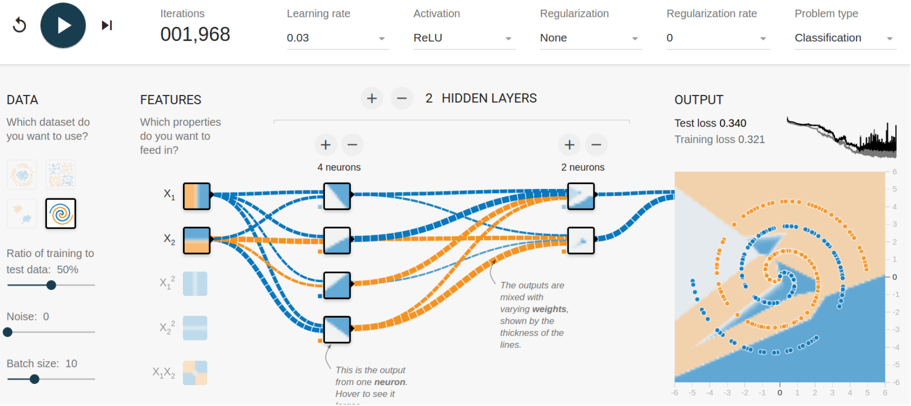
OUTPUT

Test loss 0.416

Training loss 0.302

(http://playground.tensorflow.org)

Complex Target Function, Two Hidden Layers, ReLU



Iterations
001,968

Learning rate
0.03

Activation
ReLU

Regularization
None

Regularization rate
0

Problem type
Classification

DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

FEATURES

Which properties do you want to feed in?

2 HIDDEN LAYERS

4 neurons

2 neurons

OUTPUT

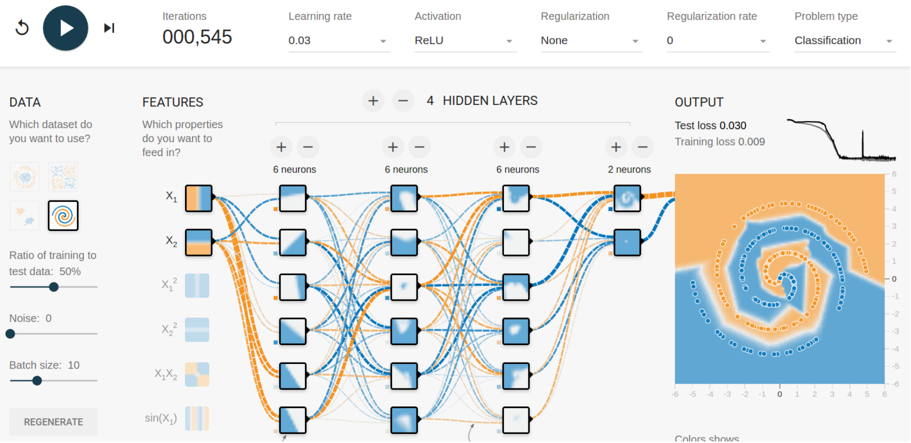
Test loss 0.340
Training loss 0.321

*The outputs are mixed with varying **weights**, shown by the thickness of the lines.*

*This is the output from one **neuron**. Hover to see it*

(http://playground.tensorflow.org)

Complex Target Function, Four Hidden Layers, ReLU



Iterations 000,545

Learning rate 0.03

Activation ReLU

Regularization None

Regularization rate 0

Problem type Classification

DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

FEATURES

Which properties do you want to feed in?

4 HIDDEN LAYERS

6 neurons

6 neurons

6 neurons

2 neurons

OUTPUT

Test loss 0.030

Training loss 0.009

Colors shows

(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

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

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 $\boldsymbol{\theta} := \{(\boldsymbol{W}^{(\ell)}, \boldsymbol{b}^{(\ell)})\}_{\ell=1}^{L+1}$ 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...)

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

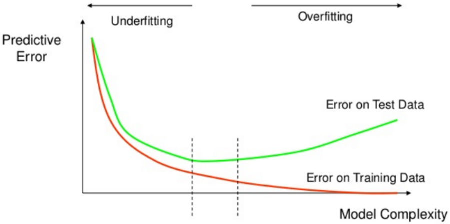
3. Conclusions

Empirical Risk Minimization

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

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

- $\Omega(\boldsymbol{\theta})$ is a regularizer
- $L(\boldsymbol{f}(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i)$ 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:

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

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

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:

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

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

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

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

Stochastic Gradient Descent with Mini-Batches

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

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

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

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

The Key Ingredients of SGD

In sum, we need the following ingredients:

- The loss function $L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$;
- A procedure for computing the gradients $\nabla_{\boldsymbol{\theta}} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$;
- The regularizer $\Omega(\boldsymbol{\theta})$ 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 $\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}) \approx \boldsymbol{y}$
- We minimize the mean squared error:

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

- Loss gradient:

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

Negative Log-Likelihood (Cross-Entropy)

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

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

where $\boldsymbol{z}$ is the output pre-activation.

- Loss gradient at output pre-activation:

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

Sparsemax Loss (Martins and Astudillo, 2016)

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

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

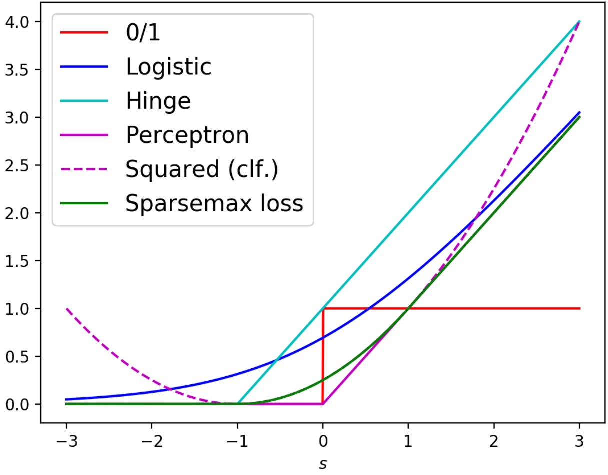
  where $\boldsymbol{z}$ is the output pre-activation, $S(\boldsymbol{z})$ is the support of $p(y \mid \boldsymbol{x})$ and $\tau^2 : \mathbb{R}^K \to \mathbb{R}$ is the square of the threshold function (see Martins and Astudillo (2016) for details).

- Loss gradient at output pre-activation:

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

Classification Losses in Two Dimensions

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



The Key Ingredients of SGD

In sum, we need the following ingredients:

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

Outline

1. Neural Networks
    - Definition
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    - Universal Approximation

2. **Training Neural Networks**
    - Empirical Risk Minimization
    - Gradient Backpropagation
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3. Conclusions

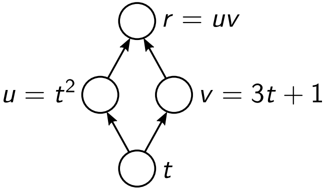
Gradient Computation

- Recall that we need to compute

$$\nabla_{\boldsymbol{\theta}} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$$

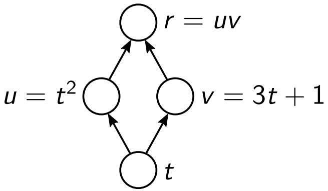
  for $\boldsymbol{\theta} = \{(\boldsymbol{W}^{(\ell)}, \boldsymbol{b}^{(\ell)})\}_{\ell=1}^{L+1}$ (the weights and biases at all layers)
- This will be done with the gradient backpropagation algorithm
- **Key idea:** use the chain rule for derivatives!

Recap: Chain Rule



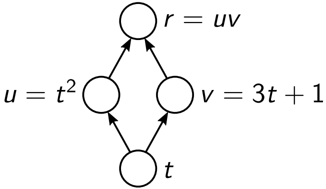
$$\frac{\partial r(t)}{\partial t} \quad = \quad ?$$

Recap: Chain Rule



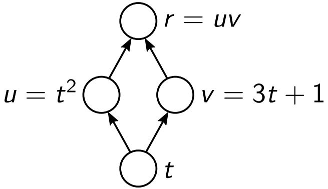
$$\frac{\partial r(t)}{\partial t} = \frac{\partial r(u)}{\partial u}\frac{\partial u(t)}{\partial t} + \frac{\partial r(v)}{\partial v}\frac{\partial v(t)}{\partial t}$$

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

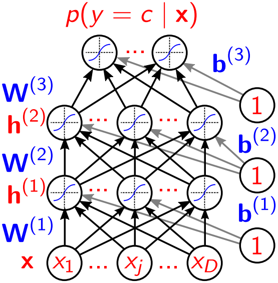
Main message: gradient backpropagation is just the chain rule of derivatives!

Hidden Layer Gradient

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

$$\frac{\partial L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}),y)}{\partial h_j^{(\ell)}} = \sum_i \frac{\partial L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}),y)}{\partial z_i^{(\ell+1)}} \frac{\partial z_i^{(\ell+1)}}{\partial h_j^{(\ell)}}$$

$$= \sum_i \frac{\partial L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}),y)}{\partial z_i^{(\ell+1)}} \boldsymbol{W}_{i,j}^{(\ell+1)}$$

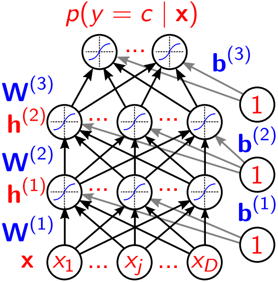


Hence $\nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}),y) = \boldsymbol{W}^{(\ell+1)^\top} \nabla_{\boldsymbol{z}^{(\ell+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}),y)$.

Hidden Layer Gradient (Before Activation)

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

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



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

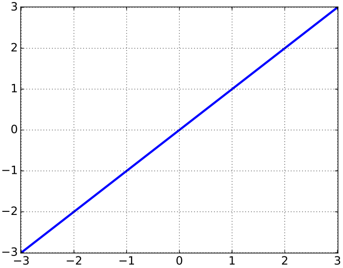
How to compute the derivative of the activation function $\boldsymbol{g}'(\boldsymbol{z}^{(\ell)})$?

Linear Activation

$$\boxed{g(z) = z}$$

Derivative:

$$\boxed{g'(z) = 1}$$

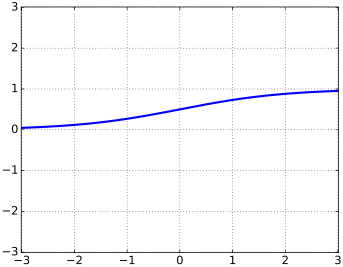


Sigmoid Activation

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

Derivative:

$$\boxed{g'(z) = g(z)(1 - g(z))}$$

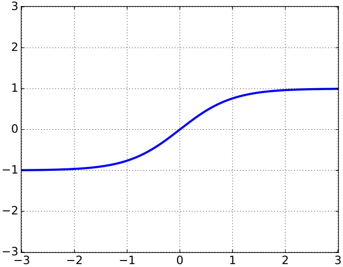


Hyperbolic Tangent Activation

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

Derivative:

$$\boxed{g'(z) = 1 - g(z)^2}$$

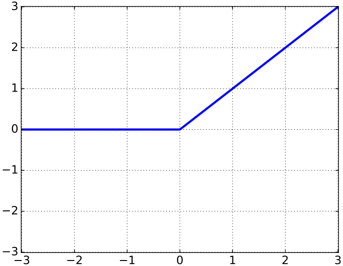


Rectified Linear Unit Activation (Glorot et al., 2011)

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

Derivative (except for $z = 0$):

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

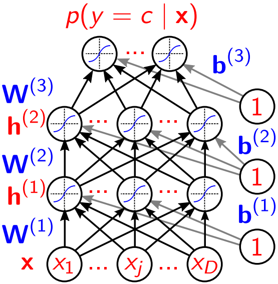


Parameter Gradient

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

$$\frac{\partial L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)}{\partial \boldsymbol{W}^{(\ell)}_{i,j}} = \frac{\partial L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)}{\partial z^{(\ell)}_i} \frac{\partial z^{(\ell)}_i}{\partial \boldsymbol{W}^{(\ell)}_{i,j}}$$

$$= \frac{\partial L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)}{\partial z^{(\ell)}_i} h^{(\ell-1)}_j$$



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

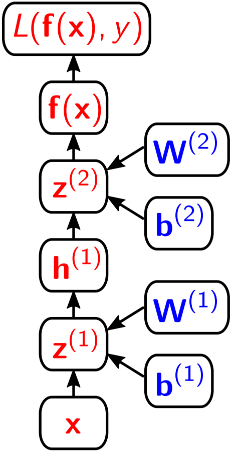
Similarly, $\nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$

Backpropagation

```
Compute output gradient (before activation):
    $\nabla_{\boldsymbol{z}^{(L+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = -(\mathbf{1}_y - \boldsymbol{f}(\boldsymbol{x}))$
for $\ell$ from $L+1$ to $1$ do
    Compute gradients of hidden layer parameters:
        $\nabla_{\boldsymbol{W}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)\ \boldsymbol{h}^{(\ell-1)^\top}$
        $\nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$
    Compute gradient of hidden layer below:
        $\nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \boldsymbol{W}^{(\ell+1)^\top} \nabla_{\boldsymbol{z}^{(\ell+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$
    Compute gradient of hidden layer below (before activation):
        $\nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \odot \boldsymbol{g}'(\boldsymbol{z}^{(\ell)})$
end for
```

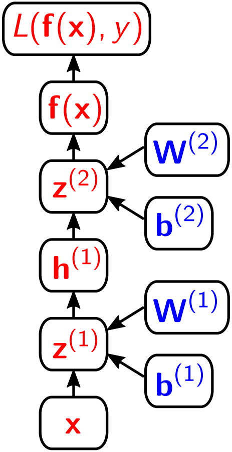
Computation Graph

- 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

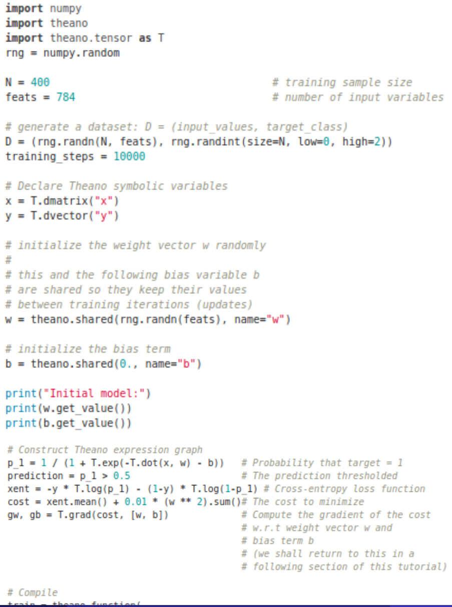
- Theano
- Tensorflow
- Torch, Pytorch
- MXNet
- Keras
- Caffe
- DyNet
- ...

All implement automatic differentiation.

We will have a Pytorch tutorial next class (TA guest lecture)

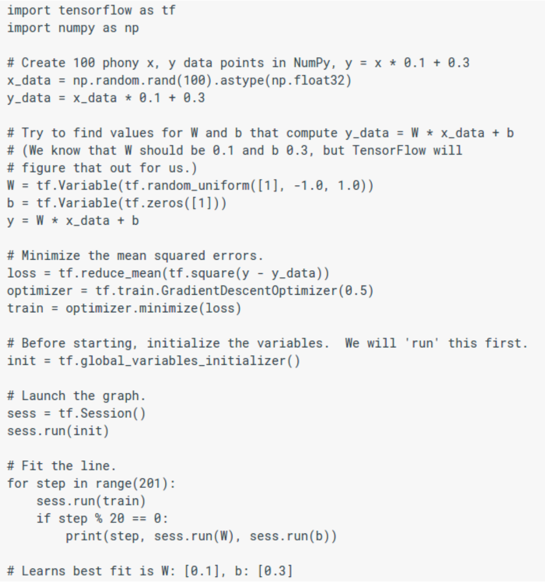
Please bring your laptops!

Some Theano Code (Logistic Regression)



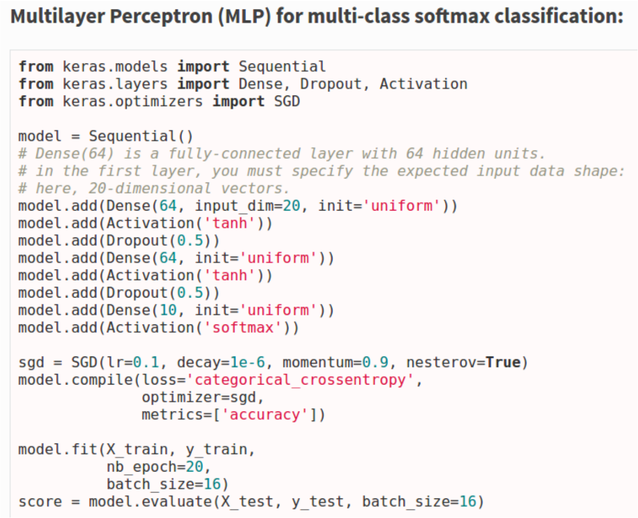
```python
import numpy
import theano
import theano.tensor as T
rng = numpy.random

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(
```

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

Regularization

Recall that we're minimizing the following objective function:

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

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)

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

- Gradient is:

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

- This has the effect of a weight decay:

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

ℓ_1 Regularization

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

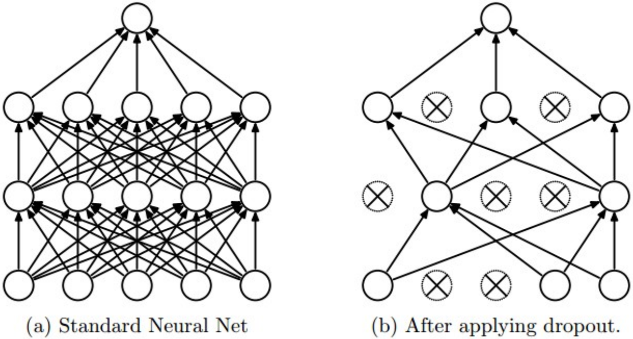
$$\Omega(\boldsymbol{\theta}) = \sum_{\ell} \|\boldsymbol{W}^{(\ell)}\|_1$$

- Gradient is:

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

- 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 $\ell = 1, \ldots, L$):

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

- 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):
    $$\nabla_{\boldsymbol{z}^{(L+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = -(\mathbf{1}_y - \boldsymbol{f}(\boldsymbol{x}))$$
for $\ell$ from $L+1$ to 1 do
    Compute gradients of hidden layer parameters:
        $$\nabla_{\boldsymbol{W}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \underbrace{\boldsymbol{h}^{(\ell-1)^\top}}_{\text{includes } \boldsymbol{m}^{(\ell-1)}}$$
        $$\nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$
    Compute gradient of hidden layer below:
        $$\nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \boldsymbol{W}^{(\ell+1)^\top} \nabla_{\boldsymbol{z}^{(\ell+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$
    Compute gradient of hidden layer below (before activation):
        $$\nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \odot \boldsymbol{g}'(\boldsymbol{z}^{(\ell)}) \odot \boldsymbol{m}^{(\ell-1)}$$
end for
```

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

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):

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

- 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

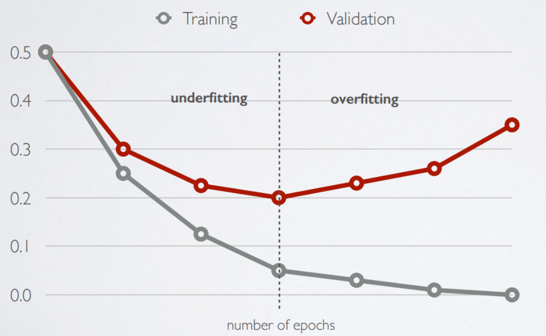
Search for the best configuration of the hyperparameters:

- 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 accross 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

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

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

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

- 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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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?

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