Feed Forward Neural Networks

A. Maier, V. Christlein, K. Breininger, S. Vesal, F. Meister, C. Liu, S. Gündel, S. Jaganathan, N. Maul, M. Vornehm, L. Reeb, F. Thamm, M. Hoffmann, C. Bergler, F. Denzinger, W. Fu, B. Geissler, Z. Yang
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May 28, 2020

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Outline

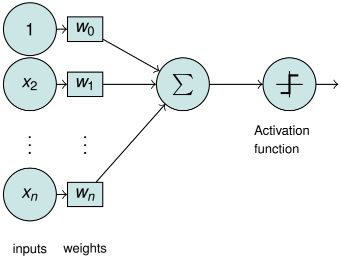
Model

Recap: Perceptrons

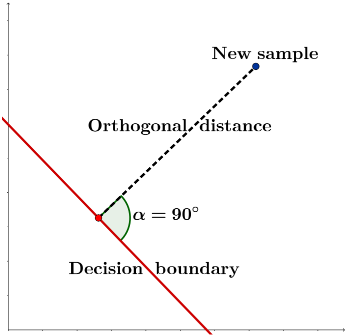
- Perceptron's decision rule:

$$\hat{y} = \mathrm{sign}(\mathbf{w}^T \mathbf{x})$$

- Classification only depends on sign of distance

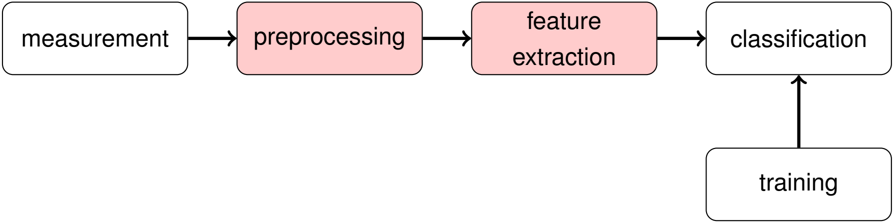


Perceptron



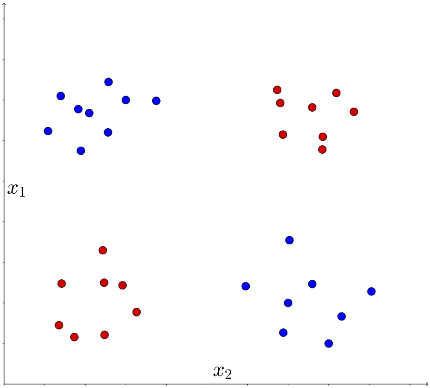
Linear decision boundary

Recap: Pattern Recognition Pipeline



- (Multi-layer) perceptron (today's lecture) still uses predefined features
- "Hand-crafted" feature design is replaced by **data driven feature learning** in state-of-the-art architectures (upcoming lectures)
- Most concepts are important across architectures!

XOR Problem

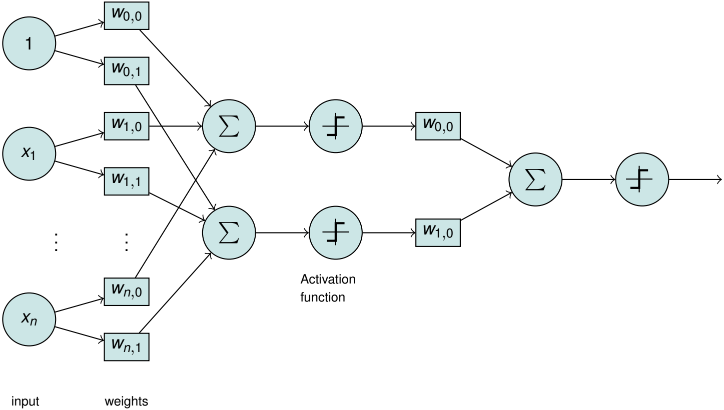


Samples from a XOR problem

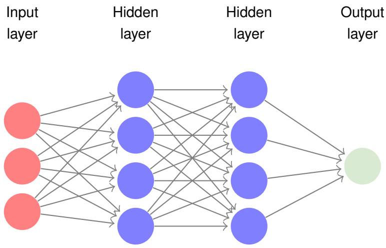
- XOR can't be solved with a line
- 1969: "Perceptrons" described limitations of neural networks
- AI funding was cut heavily
- This became known as "AI winter"

Multi-Layer Perceptron

- A perceptron resembles a single neuron
- Idea: Use multiple neurons!
- This enables non-linear decision boundaries



Terminology



- Terms: Input layer, hidden layers, output layer
- A single hidden layer (of arbitrary width) can already be shown to be a **universal function approximator**
- Non-linear functions
  - are called activation functions in hidden layers
  - predict in the output layer and are used for the loss function

Perceptrons as Universal Function Approximators

Universal Approximation Theorem

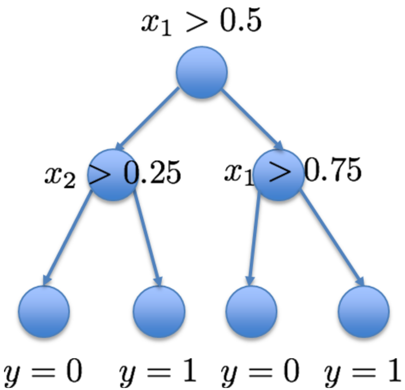
- Let $\varphi(\cdot)$ be a non-constant, bounded and monotonically increasing function.
- For any $\varepsilon > 0$ and any continuous function f defined on a compact subset of $\mathbb{R}^m$, there exist an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ where $i = 1, \ldots, N$, such that

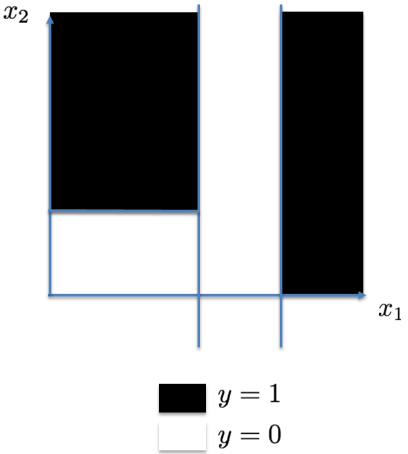
$$F(\mathbf{x}) = \sum_{i=1}^{N} v_i \varphi(\mathbf{w}_i^T \mathbf{x} + b_i) \quad \text{with}$$

$$|F(\mathbf{x}) - f(\mathbf{x})| < \varepsilon$$

$\rightarrow$ We can approximate *any function with just one hidden layer* with a sensible activation function.

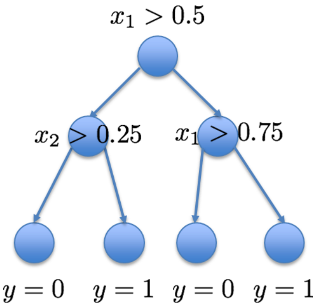
Classification Trees: Why do we need a universal approximator?

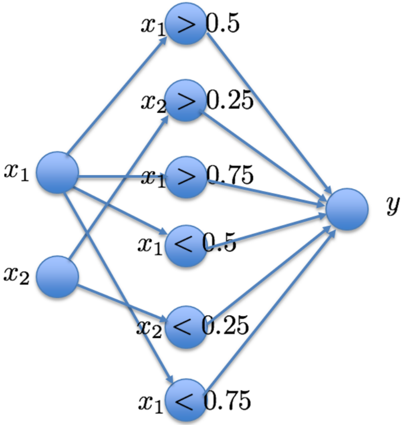




We can transform this into a network!

Classification Trees: Why do we need a universal approximator?





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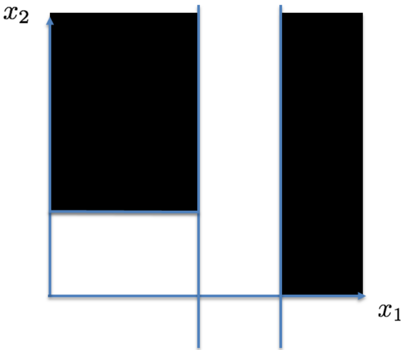

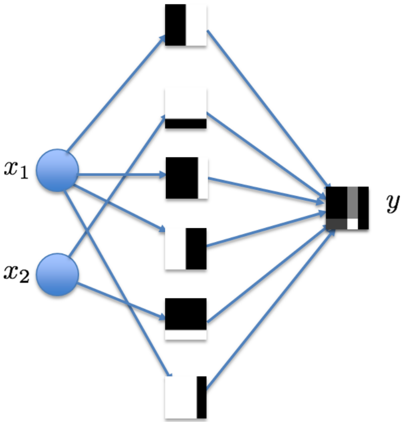

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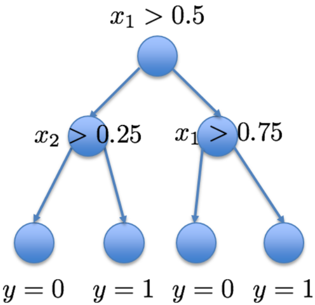

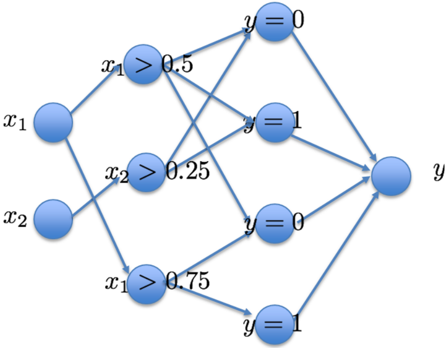

Universal Approximation Theorem

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$$F(\mathbf{x}) = \sum_{i=1}^{N} v_i \varphi(\mathbf{w}_i^T \mathbf{x} + b_i) \quad \text{with}$$

$$|F(\mathbf{x}) - f(\mathbf{x})| < \varepsilon$$

$\rightarrow$ We can approximate *any function with just one hidden layer* with a sensible activation function.

$\rightarrow$ **We have no idea *how*: how many nodes, how to train, ...**

NEXT TIME

ON DEEP LEARNING

Feed Forward Neural Networks - Part 2

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From Activations to Classifications: Softmax Function

Terminology

- So far: ground truth/estimated label is described by $y/\hat{y} \in \{-1, 1\}$.
- Instead, we can use a vector $\mathbf{y} = (y_1, \ldots, y_K)^T$ where $K = \#$classes.
- For exclusive classes, **y** looks as follows:

$$y_k = \begin{cases} 1 & \text{if } k \text{ is the index of the true class,} \\ 0 & \text{otherwise} \end{cases}$$

- Called **one-hot encoding**: Only one element is $\neq 0$.
- Classifier output $\hat{\mathbf{y}}$ can represent class probabilities.
- Better descriptor, especially for multi-class problems!

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- $\hat{\mathbf{y}}$ has two properties:
  1. $\sum_{k=1}^{K} \hat{y}_k = 1$
  2. $\hat{y}_k \geq 0 \quad \forall \hat{y}_k \in \hat{\mathbf{y}}$
- These are two of Kolmogorov's axioms for a probability distribution.
- This allows to treat the output as normalized probabilities.
- The softmax function is also known as the normalized exponential function.

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- Example: three-~~three~~four-class problem

Label	x_k	$\exp(x_k)$	$\hat{y}_k$
Tiger	-3.44	0.03	0.0006
Airplane	1.16	3.19	0.0596
Boat	-0.81	0.44	0.0083
Heavy Metal	3.91	49.90	0.9315

Loss functions

- The cross entropy H of probability distributions **p** and **q**

$$\mathrm{H}(\mathbf{p}, \mathbf{q}) = -\sum_{k=1}^{K} p_k \log(q_k)$$

- Based on H, we formulate a loss function L:

$$L(\mathbf{y}, \hat{\mathbf{y}}) = -\log(\hat{y}_k)\big|_{y_k=1}$$

- We will talk more about this during the next session!

"Softmax loss"

- Cross-entropy and the Softmax function typically appear together

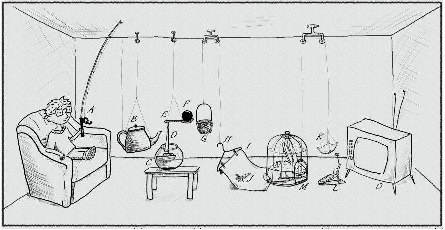
$$L(\mathbf{y}, \mathbf{x}) = -\log\left(\frac{\exp(x_k)}{\sum_{j=1}^{K}\exp(x_j)}\right)\Big|_{y_k=1}$$

- One-hot encoding very convenient ➔represents a histogram
- Naturally handles multiple class problems

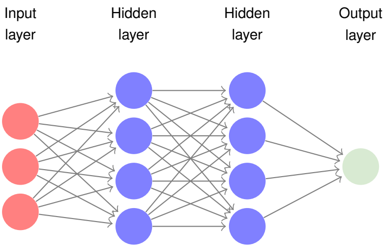
Optimization

Credit Assignment Problem

- What do those two images have in common?



Source: https://krypt3ia.files.wordpress.com/2011/11/rube.jpg



- If it doesn't work it's hard to know which parts to adjust.

Formalization as Optimization Problem

Goal: Find optimal weights $\mathbf{w}$ for all layers:

- Abstract the whole network as a function:

$$L(\mathbf{w}, \mathbf{x}, \mathbf{y})$$

- Consider all M training samples:

$$\mathbb{E}_{\mathbf{x},\mathbf{y} \sim \hat{p}_{\text{data}}(\mathbf{x},\mathbf{y})}\left[L(\mathbf{w}, \mathbf{x}, \mathbf{y})\right] = \frac{1}{M} \sum_{m=1}^{M} L(\mathbf{w}, \mathbf{x}, \mathbf{y})$$

- We now know what to do:

$$\underset{\mathbf{w}}{\text{minimize}} \quad \left\{L(\mathbf{w}, \mathbf{x}, \mathbf{y})\right\}$$

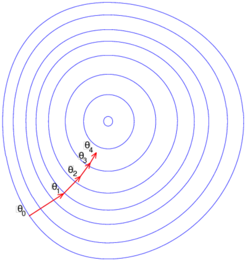
Gradient Descent

$$\underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \frac{1}{M} \sum_{m=1}^{M} L(\mathbf{w}, \mathbf{x}, \mathbf{y}) \right\}$$

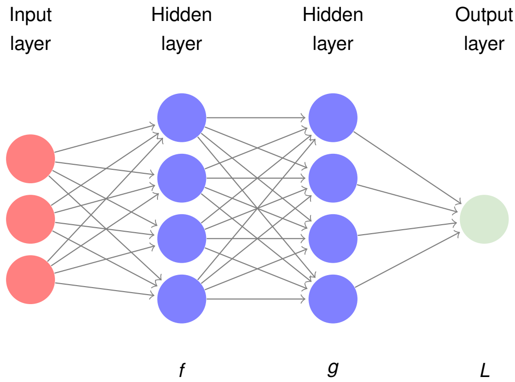
- Method of choice: Gradient Descent
  1. Initialize **w**
  2. Iterate until convergence:

$$\mathbf{w}^{k+1} = \mathbf{w}^{k} - \eta \nabla_{\mathbf{w}} \frac{1}{M} \sum_{m=1}^{M} L(\mathbf{w}, \mathbf{x}, \mathbf{y})$$

  3. η is commonly referred to as the **learning rate**



What is this L we are trying to optimize?



- Complex network can be seen as composed functions:

$$L(\mathbf{w}, \mathbf{x}, \mathbf{y}) = L(g(f(\mathbf{x}, \mathbf{w}_f), \mathbf{w}_g), \mathbf{y})$$

NEXT TIME

ON DEEP LEARNING

Feed Forward Neural Networks - Part 3

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How to Calculate Derivatives in Complex Neural Networks?

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

Two algorithms:

- Finite differences
- Analytic derivative

Finite Differences

Definition of derivative:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Due to finite precision the symmetric definition is preferred:

$$f'(x) = \lim_{h \to 0} \frac{f\left(x+\frac{1}{2}h\right)-f\left(x-\frac{1}{2}h\right)}{h}$$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

$$f'(x) = \lim_{h \to 0} \frac{f\left(x + \frac{1}{2}h\right) - f\left(x - \frac{1}{2}h\right)}{h}$$

Let's calculate it:

- Set h to $2 \cdot 10^{-2}$

$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\left(\left(2\left(1 + 10^{-2}\right) + 9\right)^2 + 3\right) - \left(\left(2\left(1 - 10^{-2}\right) + 9\right)^2 + 3\right)}{2 \cdot 10^{-2}}$$

$$= \frac{(124.4404 - 123.5604)}{2 \cdot 10^{-2}}$$

$$= 43.9999$$

Finite Differences Summed up

- For practical use it often suffices to use $h = 1 \cdot 10^{-5}$
- For a more accurate derivative [7] use: $h = \epsilon_f^{\frac{1}{3}} \cdot x_c$
  - Where $\epsilon_f \approx 10^{-7}$
  - The characteristic scale is approximated as $x_c = x$
  - Prevent division by zero at $x = 0$

Conclusion

- **Easy** to use
- We only need to be able to **evaluate** functions
- Computationally **inefficient**
- **Frequently used** to check implementations

Analytic gradient

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

Four analytic rules:

1. $\frac{d}{dx}\text{const} = 0$
2. Linearity: $\frac{d}{dx}$ is a linear operator
3. Monomials: $\frac{d}{dx} x^n = n \cdot x^{n-1}$
4. Chain rule: $\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \frac{d}{dx} g(x)$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

1. $\frac{d}{dx}\text{const} = 0$
2. $\frac{d}{dx}$ is linear
3. $\frac{d}{dx}x^n = n \cdot x^{n-1}$
4. $\frac{d}{dx}f(g(x)) = \frac{d}{dg}f(g) \cdot \frac{d}{dx}g(x)$

Let's calculate it:

$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\partial}{\partial x_1}(2x_1 + 9)^2 \qquad \text{Rules 1 and 2}$$

$$= \frac{\partial}{\partial z}(z)^2 \frac{\partial}{\partial x_1}(2x_1 + 9) \qquad \text{Rule 4 and } 2x_1 + 9 = z$$

$$= 2(2x_1 + 9)\frac{\partial}{\partial x_1}(2x_1 + 9) \qquad \text{Rule 3}$$

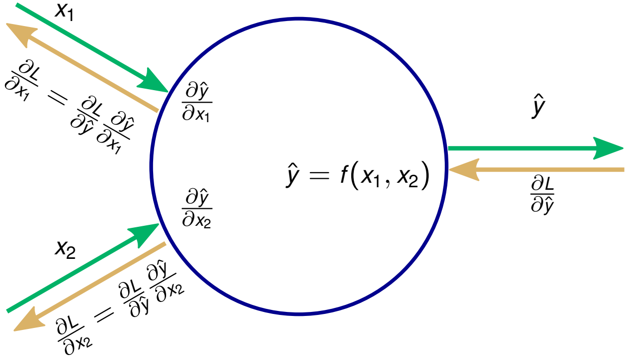
$$= 2(2x_1 + 9) \cdot 2 = 44 \qquad \text{Rules 1 and 2 and } x_1 = 1$$

Analytic Gradient Summed up

- **Chain rule** and **Linearity** enable to **decompose** complex functions
- Analytic formulas have to be calculated manually
- Computationally more **efficient** than finite differences

Can we compute analytic gradients automatically?

Backpropagation Algorithm

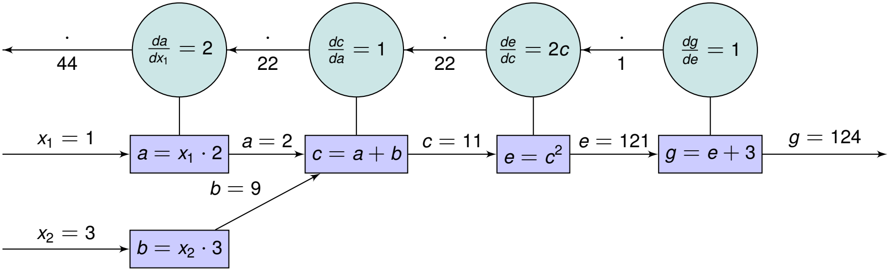


1. Forward pass: Compute activations
2. Backward pass: Recursively apply chain rule

Example Problem

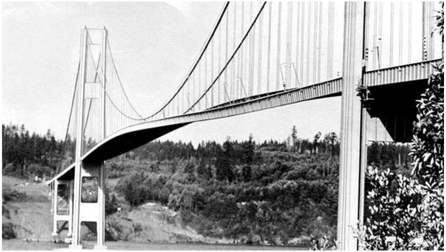
- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

$$\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \frac{d}{dx} g(x)$$

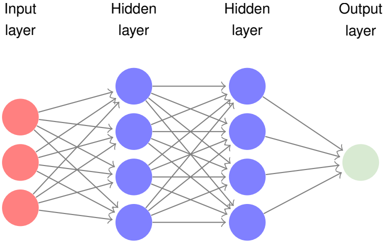


Stability Problem

- What do those two images have in common?

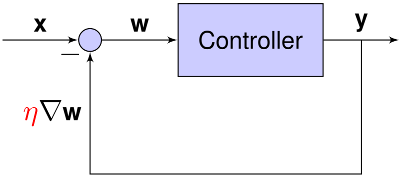


Click for video

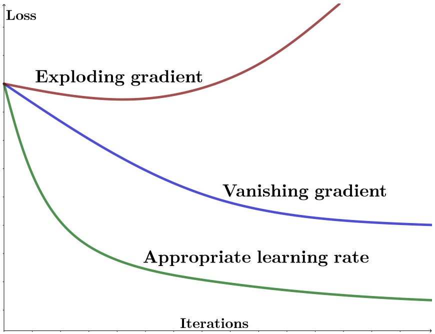


- Both suffer from positive feedback!
- This can cause disaster

Feedback loop



Analogy to control theory



- If η is too high $\rightarrow$ **positive feedback** $\rightarrow$ loss grows **without bounds**
- If η is too small $\rightarrow$ **negative feedback** $\rightarrow$ **gradient vanishes**
- Choice of η is **critical** for learning

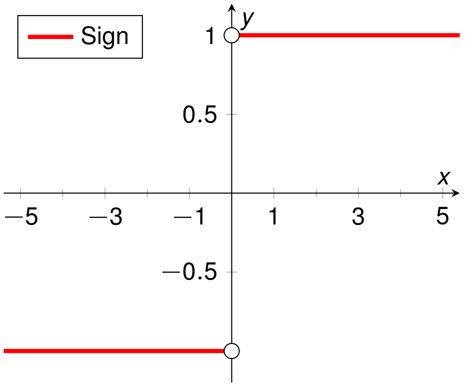
Backpropagation Summed up

- Built around the **chain rule**
- Uses a **forward-pass** through the function
- Computationally very **efficient** by using a **dynamic programming** approach
- Is **no training algorithm**, because it just computes a gradient

Consequences

- Product of partials $\rightarrow$ numerical **errors multiply**
- Product of partials $\rightarrow$ **vanishing** or **exploding** gradient

About the sign Activation Function



Sign

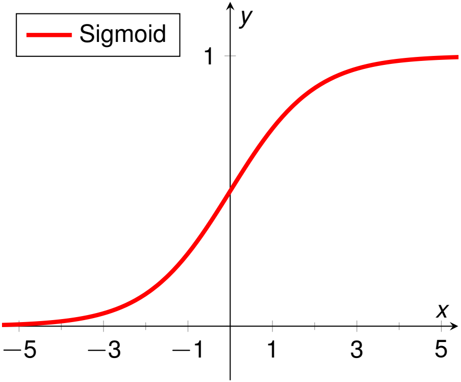
$$f(x) = \begin{cases} +1 & \text{for } x \geq 0 \\ -1 & \text{for } x < 0 \end{cases}$$

$$f'(x) = 2\delta(x)$$

\+ Normalized output

− Gradient vanishes almost everywhere!

Smooth Activation Function



Sigmoid (logistic function)

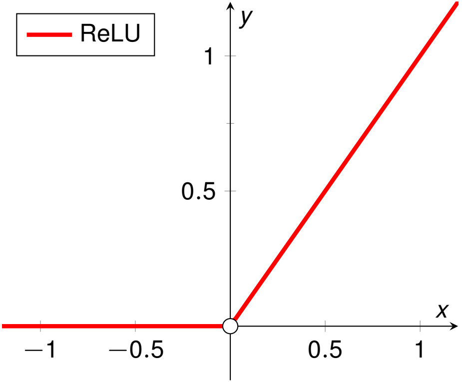
$$f(x) = \frac{1}{1 + exp(-x)}$$

$$f'(x) = f(x)(1 - f(x))$$

+ Normalized output

− Gradient still eventually vanishes

Piecewise-linear Activation Function



Rectified Linear Unit (ReLU)

$$f(x) = \max(0, x)$$

$$f'(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{else} \end{cases}$$

+ Less vanishing gradient

NEXT TIME

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Feed Forward Neural Networks - Part 4

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Layer Abstraction

ACADEMIAE FRIDERICO ALEXANDRINAE SIGILLUM

From Graphs of Nodes to Graphs of Layers

- We introduced **layers** but computed everything on individual nodes
- It is convenient to add further abstraction
- But how can we express this?

Recall: Single neuron

- Add a bias unit to $\mathbf{x} \in \mathbb{R}^{N-1}$ by adding a dimension with $x_n = 1$
- This is a connection from every input element to the single output element:

$$\hat{y} = \mathbf{w}^T \mathbf{x}$$

Representing the connections

- Assume we have M neurons $\rightarrow$ M sets of weights: $\mathbf{w}_m$ for $m \in \{1, \dots, M\}$

$$\hat{y}_m = \mathbf{w}_m^T \mathbf{x}$$

- We rewrite this operation as matrix-vector multiplication:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- This is known as **fully connected layer**.
- It represents any arbitrary connection topology between layers.
- We can describe back-propagation in this more abstract view as well!

Fully Connected Layer

$$\begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \end{pmatrix} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

- The forward-pass is:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- After the forward-pass through all layers, we can compute a loss that depends on our loss function L.
- We need two gradients for the backward-pass:
  - Gradient with respect to the weights: $\frac{\partial \mathbf{L}}{\partial \mathbf{W}}$ for gradient descend
  - Gradient with respect to the inputs: $\frac{\partial \mathbf{L}}{\partial \mathbf{x}}$ for backpropagation

Fully Connected Layer Summed up

- Can represent any connection topology
- Enables higher level view concentrating on layers instead of nodes
- Is a matrix multiplication:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- Its gradient with respect to the weights:

$$\frac{\partial L}{\partial \mathbf{W}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{W}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \mathbf{x}^T$$

- Its gradient with respect to the input:

$$\frac{\partial L}{\partial \mathbf{x}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}} = \mathbf{W}^T \frac{\partial L}{\partial \hat{\mathbf{y}}}$$

Fully Connected Layer: Simple example

- Assume we are looking at a simple network (no activation function) with the forward pass:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- We try to find parameters **W** that minimize the following loss function:

$$L(\mathbf{x}, \mathbf{W}, \mathbf{y}) = \frac{1}{2}\|\mathbf{W}\mathbf{x} - \mathbf{y}\|_2^2$$

- Then simply: $\frac{\partial L}{\partial \hat{\mathbf{y}}} = \hat{\mathbf{y}} - \mathbf{y} = \mathbf{W}\mathbf{x} - \mathbf{y}$
- The gradient with respect to the weights: $\frac{\partial L}{\partial \mathbf{W}} = (\mathbf{W}\mathbf{x} - \mathbf{y})\mathbf{x}^T$
- The gradient with respect to the inputs: $\frac{\partial L}{\partial \mathbf{x}} = \mathbf{W}^T(\mathbf{W}\mathbf{x} - \mathbf{y})$

Linear Network in Matrix notation

- Let's add some layers

$$\hat{\mathbf{y}} = \hat{\mathbf{f}}_3(\hat{\mathbf{f}}_2(\hat{\mathbf{f}}_1(\mathbf{x}))) = \mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x}$$

- Associated loss function:

$$L(\theta) = \frac{1}{2}||\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y}||_2^2$$

- Gradients?

Linear Network in Matrix notation

- Associated loss function:

$$L(\theta) = \frac{1}{2}\|\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y}\|_2^2$$

$$\hat{\mathbf{y}} = \hat{\mathbf{f}}_3(\hat{\mathbf{f}}_2(\hat{\mathbf{f}}_1(\mathbf{x}))) = \mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x}$$

- Last layer gradient

$$\frac{\partial L}{\partial \mathbf{W}_3} = \underbrace{\frac{\partial L}{\partial \hat{\mathbf{f}}_3}}_{(\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})} \underbrace{\frac{\partial \hat{\mathbf{f}}_3}{\partial \mathbf{W}_3}}_{(\mathbf{W}_2\mathbf{W}_1\mathbf{x})^T} = (\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})(\mathbf{W}_2\mathbf{W}_1\mathbf{x})^T$$

Linear Network in Matrix notation

- Associated loss function:

$$L(\theta) = \frac{1}{2} \|\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y}\|_2^2$$

$$\hat{\mathbf{y}} = \hat{\mathbf{f}}_3(\hat{\mathbf{f}}_2(\hat{\mathbf{f}}_1(\mathbf{x}))) = \mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x}$$

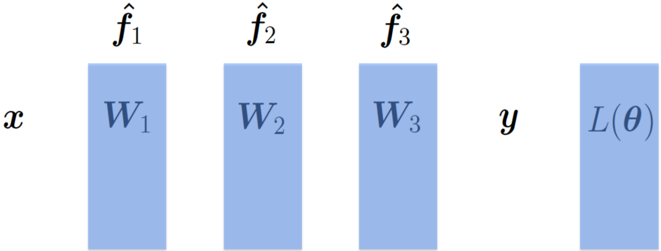
- Deeper gradients

$$\frac{\partial L}{\partial \mathbf{W}_2} = \frac{\partial L}{\partial \hat{\mathbf{f}}_3}\frac{\partial \hat{\mathbf{f}}_3}{\partial \mathbf{W}_2} = \underbrace{\frac{\partial L}{\partial \hat{\mathbf{f}}_3}}_{(\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})} \underbrace{\frac{\partial \hat{\mathbf{f}}_3}{\partial \hat{\mathbf{f}}_2}}_{(\mathbf{W}_3)^T\cdot} \underbrace{\frac{\partial \hat{\mathbf{f}}_2}{\partial \mathbf{W}_2}}_{(\mathbf{W}_1\mathbf{x})^T} = \mathbf{W}_3^T(\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})(\mathbf{W}_1\mathbf{x})^T$$

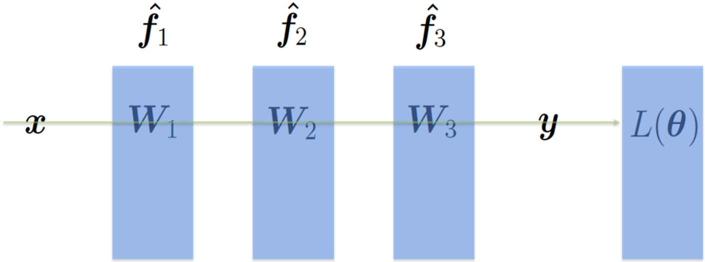
$$\frac{\partial L}{\partial \mathbf{W}_1} = \frac{\partial L}{\partial \hat{\mathbf{f}}_3}\frac{\partial \hat{\mathbf{f}}_3}{\partial \mathbf{W}_1} = \frac{\partial L}{\partial \hat{\mathbf{f}}_3}\frac{\partial \hat{\mathbf{f}}_3}{\partial \hat{\mathbf{f}}_2}\frac{\partial \hat{\mathbf{f}}_2}{\partial \mathbf{W}_1} = \underbrace{\frac{\partial L}{\partial \hat{\mathbf{f}}_3}}_{(\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})} \underbrace{\frac{\partial \hat{\mathbf{f}}_3}{\partial \hat{\mathbf{f}}_2}}_{(\mathbf{W}_3)^T\cdot} \underbrace{\frac{\partial \hat{\mathbf{f}}_2}{\partial \hat{\mathbf{f}}_1}}_{(\mathbf{W}_2)^T\cdot} \underbrace{\frac{\partial \hat{\mathbf{f}}_1}{\partial \mathbf{W}_1}}_{(\mathbf{x})^T}$$

$$= \mathbf{W}_2^T\mathbf{W}_3^T(\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})(\mathbf{x})^T$$

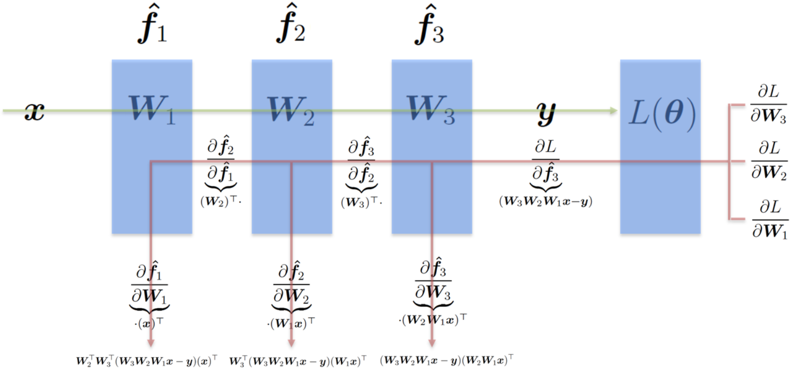
Linear Network in Matrix notation



Linear Network in Matrix notation



Linear Network in Matrix notation



Summary

- **Softmax activation** function with **cross entropy loss** mostly go together as "Softmax Loss".
- **Gradient descent** is our default training algorithm in deep learning.
- We can compute gradients using **finite differences** to check our implementation.
- We use the **backpropagation** algorithm to compute gradients efficiently.
- The **fully connected** layer is the most general connectivity between layers in a feed-forward neural network.

NEXT TIME

ON DEEP LEARNING

- Problem adapted loss functions
- Sophisticated optimization routines
- Optimization adapted to the needs of every single parameter
- An argument why neural networks shouldn't perform well
- Some very recent insights why they do perform well

Comprehensive Questions

- Name a loss function for multi-class classification in deep learning.
- Explain how this loss function works.
- How can you check if the derivative implementation of a loss function is correct?
- What does backpropagation do?
- How does backpropagation work?
- Explain the exploding and vanishing gradient problems.
- Why is the signum function not used in deep learning?

Further Reading

- Link - The original paper popularizing ReLUs
- Link - The original paper popularizing backpropagation
- Link - Bishop - Mathematical compendium for machine learning
- Link - Blog article putting backpropagation in a very general context

References

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