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Deep Learning Activation Functions

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Binary Classification and Linear Regression Problems

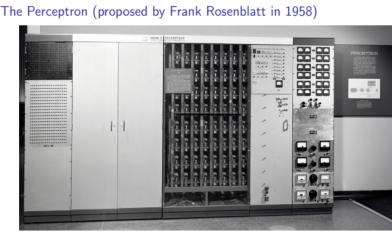
The XOR Problem

Why Do We Need Activation Functions

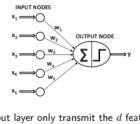
Examples of Activation Functions

Binary Classification and Linear Regression Problems

- lacktriangle In the binary classification problem, each training pair (\overline{X},y) contains feature variables $\overline{X} = (x_1, \dots x_d)$, and label y drawn from $\{-1, +1\}$.
- Variables \(X = (x_1, \ldots x_d) \), and label \(y \) drawn from \(\{ -1, +1 \} \).
 Example: Feature variables might be frequencies of words in an email, and the class variable might be an indicator of spam.
 Given labeled emails, recognize incoming spam.
 In linear regression, the dependent variable \(y \) is real-valued.
- Perceptron is designed for the binary setting.



The Perceptron: Earliest Historical Architecture



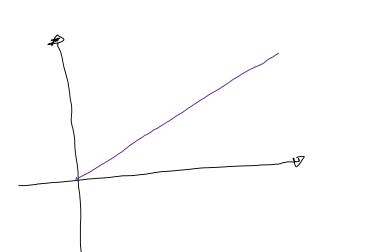
▶ The d nodes in the input layer only transmit the d features $\overline{X} = [x_1 \dots x_d]$ without performing any computation. $lackbox{ Output node multiplies input with weights } \overline{W} = [w_1 \dots w_d]$ on incoming edges, aggregates them, and applies sign activation:

What is the Perceptron Doing?

▶ Tries to find a *linear separator* $\overline{W} \cdot \overline{X} = 0$ between the two classes. lacktriangle Ideally, all positive instances (y=1) should be on the side of the separator satisfying $\overline{W} \cdot \overline{X} > 0$. lacktriangle All negative instances (y=-1) should be on the side of the separator satisfying * (emporosos entre or funces de otivosos) *

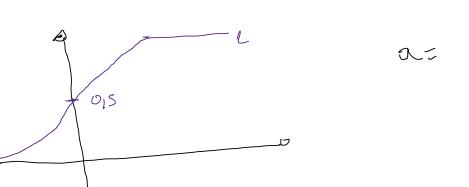
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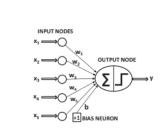
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Lourda planetos o output em binario $\hat{y} = \operatorname{sign}\{\overline{W} \cdot \overline{X}\} = \operatorname{sign}\{\sum_{}^{u} w_j x_j\}$

$$\phi(v) = \begin{cases} 1 & \text{De } v^2 \\ -1 & \text{De } v^2 \end{cases}$$

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▶ In many settings (e.g., skewed class distribution) we need an invariant part of the

prediction with bias variable b: $\hat{y} = \operatorname{sign}\{\overline{W} \cdot \overline{X} + b\} = \operatorname{sign}\{\sum w_j x_j + b\} = \operatorname{sign}\{\sum w_j x_j\}$

lackbox On setting $w_{d+1}=b$ and x_{d+1} as the input from the bias neuron, it makes little difference to learning procedures ⇒ Often implicit in architectural diagrams

Training a Perceptron

▶ Go through the input-output pairs (\overline{X},y) one by one and make updates, if predicted value \hat{y} is different from observed value $y\Rightarrow$ Biological readjustment of synaptic weights.

 $\overline{W} \Leftarrow \overline{W} + \alpha \underbrace{(y - \hat{y})} \overline{X}$

 $\overline{W} \Leftarrow \overline{W} + (2\alpha)y\overline{X}$ [For misclassified instances $y - \hat{y} = 2y$] Parameter α is the learning rate. ▶ One cycle through the entire training data set is referred to as an *epoch* ⇒ Multiple epochs required How did we derive these updates?

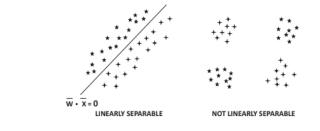
What Objective Function is the Perceptron Optimizing?

▶ At the time, the perceptron was proposed, the notion of loss function was not popular ⇒ Updates were heuristic ▶ Perceptron optimizes the perceptron criterion for *i*th training instance: $L_i = \max\{-y_i(\overline{W}\cdot\overline{X_i}), 0\}$

- Loss function tells us how far we are from a desired solution \Rightarrow Perceptron criterion is 0 when $\overline{W}\cdot \overline{X_i}$ has same sign as y_i . ▶ Perceptron updates use *stochastic gradient descent* to optimize the loss function and reach the desired outcome.

- Updates are equivalent to $\overline{W} \Leftarrow \overline{W} - \alpha \left(\frac{\partial L_i}{\partial w_1} \dots \frac{\partial L_i}{\partial w_d} \right)$

Where does the Perceptron Fail?



The perceptron fails at similar problems as a linear SVM Classical solution: Feature engineering with Radial Basis Function network ⇒ Similar to kernel SVM and good for noisy data
 Deep learning solution: Multilayer networks with nonlinear activations ⇒ Good for data with a lot of structure

The XOR Problem

"Perceptrons" by Marvin Minsky and Seymour Papert (1969). Perceptrons cannot solve the XOR problem. ▶ Significant decline in interest and funding of neural network research. -, lorde de folhe de perception sièverages atronaurel son den son Je 500 función de strong como o do XOR

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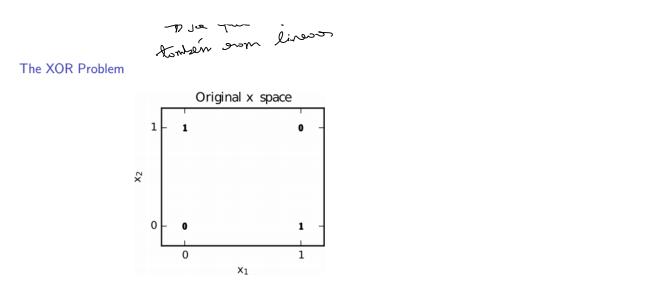
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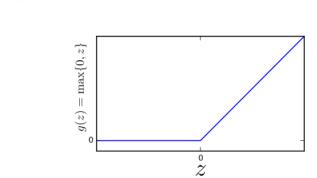
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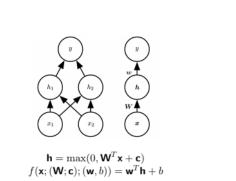
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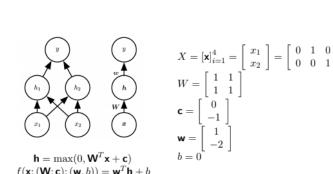
Rectified Linear Activation



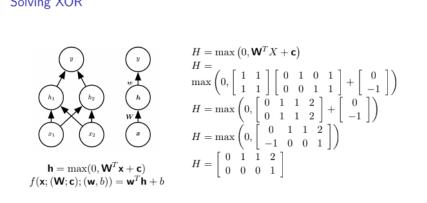
Network Diagrams

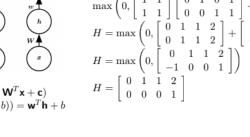


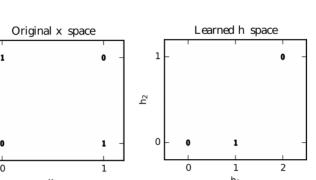
Solving XOR

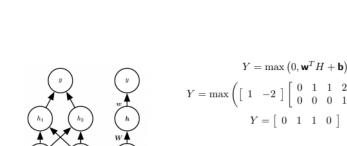


Solving XOR









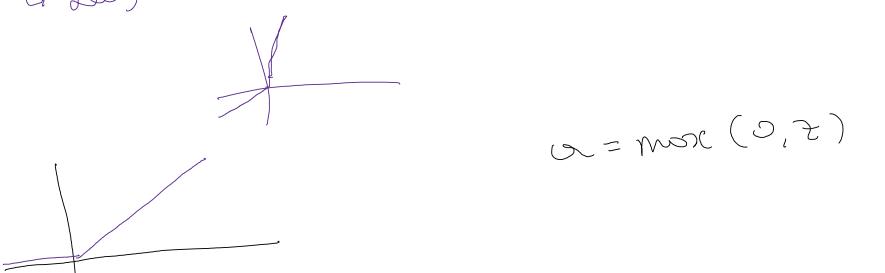
 $\begin{aligned} \mathbf{h} &= \max(0, \mathbf{W}^T \mathbf{x} + \mathbf{c}) \\ f(\mathbf{x}; (\mathbf{W}; \mathbf{c}); (\mathbf{w}, b)) &= \mathbf{w}^T \mathbf{h} + b \end{aligned}$

- transformation. Very close to linear.
- Sufficient to represent any function if enough hidden units are connected.
- Why ReLU is so effective? Strong gradient. Gradient descent can compute large gradients.

- Activation functions required for inference may be different from those used in loss functions in training. - Perceptron uses sign function $\Phi(v) = \operatorname{sign}(v)$ for prediction but does not use any activation for computing the perceptron criterion (during training).
- Why Do We Need Loss Functions?
- ▶ The loss function is typically paired with the activation function to quantify how far we are from a desired result. An example is the perceptron criterion.
- $L_i = \max\{-y(\overline{W}\cdot\overline{X}), 0\}$ Note that loss is 0, if the instance (\(\overline{X}\), y) is classified correctly.
- ▶ Even though many machine learning problems have discrete outputs, a smooth and continuous loss function is required to enable gradient-descent procedures. ► Gradient descent is at the heart of neural network parameter learning.
- Nonlinearity. Continuously differentiable.
- Range. Monotonicity.
- Smooth. Approximating identity near the origin.

Summary

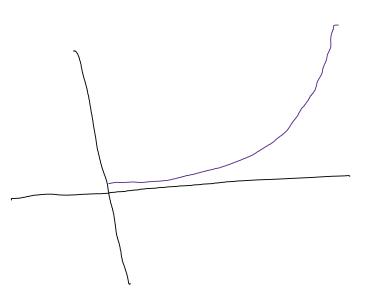
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- Rectified Linear Activation (ReLU) ▶ Applying this function to the output of a linear transformation yields a nonlinear
- Very simple nonlinearity (2 pieces piecewise-linear). Default activation function recommended for use with most feedforward NNs.
- Consistent behavior across its whole domain. Historical reasons.
- Why Do We Need Activation Functions?
- Why Do We Need Activation Functions?
 A neural network with any number of layers but only linear activations can be shown to be equivalent to a single-layer network.
 ▶ An activation function Φ(v) in the output layer can control the nature of the output (e.g., probability value in [0,1])
- output (e.g., probability value in $\left[0,1\right]$) In *multilayer* neural networks, activation functions bring nonlinearity into hidden layers, which increases the complexity of the model.

Examples of Activation Functions

Identity Activation

- \blacktriangleright Identity activation $\Phi(v)=v$ is often used in the output layer, when the outputs are real values.
- lacktriangle For a single-layer network, if the training pair is (\overline{X},y) , the output is as follows: $\hat{y} = \Phi(\overline{W} \cdot \overline{X}) = \overline{W} \cdot \overline{X}$
- ▶ Use of the squared loss function $(y \hat{y})^2$ leads to the *linear regression* model with numeric outputs and *Widrow-Hoff learning* with binary outputs. Identity activation can be combined with various types of loss functions (e.g., perceptron criterion) even for discrete outputs.

Summary

Examples of Activation Functions

Sign Activation

```
 \Phi(v) = \left\{ \begin{array}{ll} +1 & \text{if } v > 0; \\ -1 & \text{if } v < 0. \end{array} \right.
```

- Can be used to map to binary outputs at prediction time.
- Its non-differentiability prevents its use for creating the loss function at training time.
- Eg. while the perceptron uses the sign function for prediction, in training it requires only the linear activation.

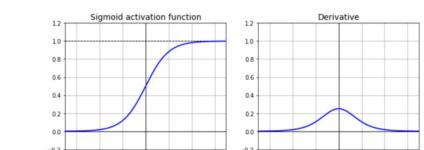
Examples of Activation Functions

Sigmoid Activation

- ▶ Sigmoid activation is defined as $\Phi(v) = 1/(1 + \exp(-v))$.
- lacktriangle For a training pair (\overline{X},y) , one obtains the following prediction in a single-layer $\hat{y} = 1/(1 + \exp(-\overline{W} \cdot \overline{X}))$
- Prediction is the *probability* that class label is +1.

 Paired with *logarithmic loss*, which $-\log(\hat{y})$ for positive instances and $-\log(1-\hat{y})$ for negative instances. $-\mathcal{L}(\hat{y},y) = -[y\log(\hat{y}) + (1-y)\log(1-\hat{y})]$
- ▶ Resulting model is *logistic regression*.

Sigmoid Activation



Sigmoid Activation

Characteristics:

► The function is a common S-shaped curve. ▶ The output of the function is centered at 0.5 with a range from 0 to 1.

► The function is monotonic but the function's derivative is not.

► The function is differentiable. That means we can find the slope of the sigmoid curve at any two points.

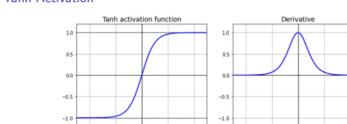
Sigmoid Activation

Drawbacks:

Vanishing gradient. Computationally expensive.The output is not zero-centered.

Examples of Activation Functions

Tanh Activation



▶ The tanh activation is a scaled and translated version of sigmoid activation. $\tanh(v) = \frac{e^{2v} - 1}{e^{2v} + 1} = 2 \cdot \operatorname{sigmoid}(2v) - 1$

Often used in hidden layers of multilayer networks

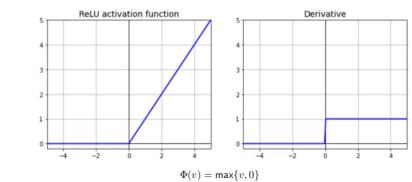
Tanh Activation

- The function is a common S-shaped curve as well. The difference is that the output of Tanh is zero centered with a range from −1 to +1 (instead of 0 to 1 in the case of the Sigmoid function).
 The same as the Sigmoid, this function is differentiable.
- ▶ The same as the Sigmoid, the function is monotonic, but the function's derivative

Summary

Examples of Activation Functions

Piecewise Linear Activation Functions - ReLU



▶ Piecewise linear activation functions are easier to train than their continuous

Piecewise Linear Activation Functions – ReLU

► Graphically, the ReLU function is composed of two linear pieces to account for

- ▶ The ReLU function is continuous, but it is not differentiable because its derivative
- is 0 for any negative input. The output of ReLU does not have a maximum value (It is not saturated) and this helps Gradient Descent.
- The function is very fast to compute.

Piecewise Linear Activation Functions – ReLU

Dying ReLU.

Examples of Activation Functions

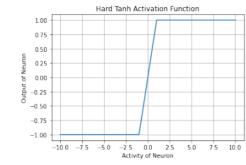
Piecewise Linear Activation Functions - Leaky ReLU

Where typically: $\gamma = 0.01$.

Summary

Examples of Activation Functions

Piecewise Linear Activation Functions – Hard TANH

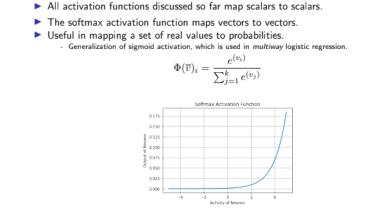


 $\Phi(v) = \max\left\{\min\left[v,1\right],-1\right\}$

Examples of Activation Functions

Softmax Activation Function

► All activation functions discussed so far map scalars to scalars.



Derivatives of Activation Functions

Neural network learning requires gradient descent of the loss.

lacktriangle Loss is often a function of the output o, which is itself obtained by using the activation function: $o = \Phi(v)$

 \blacktriangleright Therefore, we often need to compute the partial derivative of o with respect to vduring neural network parameter learning. lacktriangle Many derivatives are more easily expressed in terms of the output o rather than

Useful Derivatives

- ▶ Sigmoid: $\frac{\partial o}{\partial v} = o(1 o)$
- ▶ Tanh: $\frac{\partial o}{\partial v} = 1 o^2$ ▶ ReLU: Derivative is 1 for positive values of v and 0 otherwise.
 ▶ Hard Tanh: Derivative is 1 for $v \in (-1,1)$ and 0 otherwise.

Output Types

| Output Type | Output distribution | Out. Layer Act. Func. | Cost Function |
|-------------|---------------------|-----------------------|------------------------|
| Binary | Bernoulli | Sigmoid | Binary cross-entropy |
| Discrete | Multinoulli | Softmax | Discrete cross-entropy |
| Continuous | Gaussian | Linear | MSE |
| Continuous | Arbitrary | GAN, VAE, FVBN | Various |

Using Activation Functions

The nature of the activation in output layers is often controlled by the nature of output

 Identity activation for real-valued outputs, and sigmoid/softmax for binary/categorical outputs.
 Softmax almost exclusively for output layer and is paired with a particular type of cross-entropy loss.

 Hidden layer activations are almost always nonlinear and often use the same activation function over the entire network.

 Tanh often (but not always) preferable to sigmoid.
 ReLU has largely replaced tanh and sigmoid in many applications.

Why are Hidden Layers Nonlinear?

- A multi-layer network that uses only the identity activation function in all its layers reduces to a single-layer network that performs linear regression. $\overline{h}_1 = \Phi(W_1^T \overline{x}) = W_1^T \overline{x}$ $\overline{h}_{p+1} = \Phi(W_{p+1}^T \overline{h}_p) = W_{p+1}^T \overline{h}_p \ \, \forall p \in \{1 \dots k-1\}$ $\overline{o} = \Phi(W_{k+1}^T \overline{h}_k) = W_{k+1}^T \overline{h}_k$
- ▶ We can eliminate the hidden variable to get a simple linear relationship: $\overline{o} = W_{k+1}^T W_k^T \dots W_1^T \overline{x}$ $= (W_1 W_2 \dots W_{k+1})^T \overline{x}$
- $=\underbrace{(W_1W_2\dots W_{k+1})^T}_{W_{xo}^T}\overline{x}$
- lacktriangle We get a *single-layer* network with matrix W_{xo} .

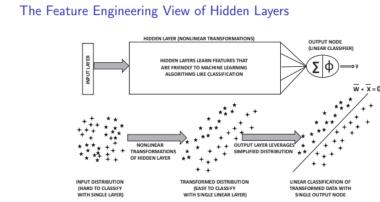
Role of Hidden Layers

- Nonlinear hidden layers perform the role of hierarchical feature engineering.

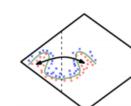
 Early layers learn primitive features and later layers learn more complex features
 Image data: Early layers learn elementary edges, the middle layers contain complex features like honeycombs, and later layers contain complex features like a part of a face.
 Deep learners are masters of feature engineering.

 The final output layer is often able to perform inference with transformed features in penultimate layer relatively easily.
 Perceptron: Cannot classify linearly inseparable data but can do so with

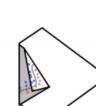
nonlinear hidden layers.



► Early layers play the role of feature engineering for later layers.







Thank you! tvieira@ic.ufal.br