Deep Learning

Activation Functions

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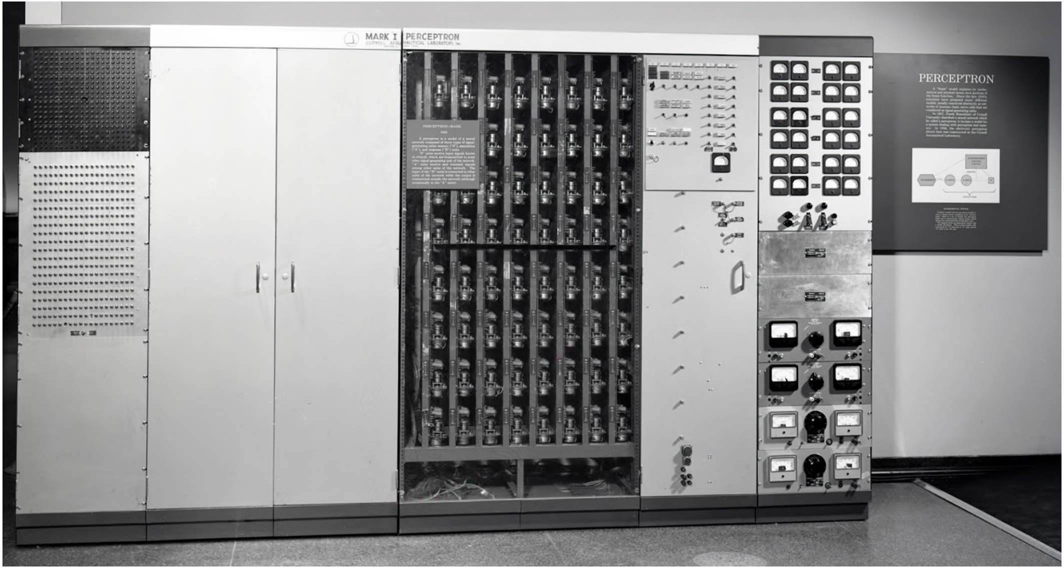
Summary

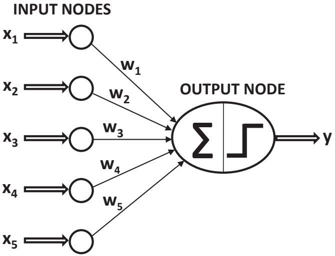
Binary Classification and Linear Regression Problems

- In the binary classification problem, each training pair $(\overline{X}, y)$ contains feature variables $\overline{X} = (x_1, \ldots x_d)$, 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.
  - Feature variables are frequencies of words in a Web page, and the dependent variable is a prediction of the number of accesses in a fixed period.
- Perceptron is designed for the binary setting.

The Perceptron (proposed by Frank Rosenblatt in 1958)



The Perceptron: Earliest Historical Architecture



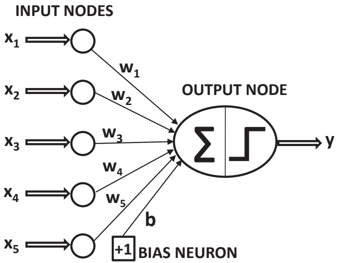
- The d nodes in the input layer only transmit the d features $\overline{X} = [x_1 \ldots x_d]$ without performing any computation.
- Output node multiplies input with weights $\overline{W} = [w_1 \ldots w_d]$ on incoming edges, aggregates them, and applies *sign activation*:

$$\hat{y} = \text{sign}\{\overline{W} \cdot \overline{X}\} = \text{sign}\{\sum_{j=1}^{d} w_j x_j\}$$

What is the Perceptron Doing?

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

Bias Neurons



- In many settings (e.g., skewed class distribution) we need an invariant part of the prediction with bias variable b:

$$\hat{y} = \text{sign}\{\overline{W} \cdot \overline{X} + b\} = \text{sign}\{\sum_{j=1}^{d} w_j x_j + b\} = \text{sign}\{\sum_{j=1}^{d+1} w_j x_j\}$$

- On setting $w_{d+1} = b$ and x_{d+1} as the input from the bias neuron, it makes little difference to learning procedures $\Rightarrow$ 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.

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

$$\overline{W} \Leftarrow \overline{W} + (2\alpha) y \overline{X} \text{ [For misclassified instances } y - \hat{y} = 2y\text{]}$$

- Parameter α is the learning rate.
- One cycle through the entire training data set is referred to as an *epoch* $\Rightarrow$ Multiple epochs required
- How did we derive these updates?

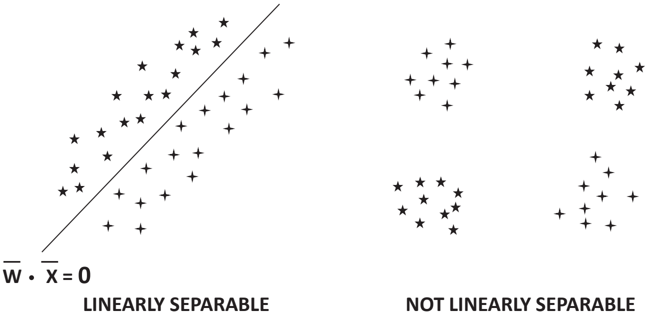
What Objective Function is the Perceptron Optimizing?

- At the time, the perceptron was proposed, the notion of loss function was not popular $\Rightarrow$ Updates were heuristic
- Perceptron optimizes the perceptron criterion for ith 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?

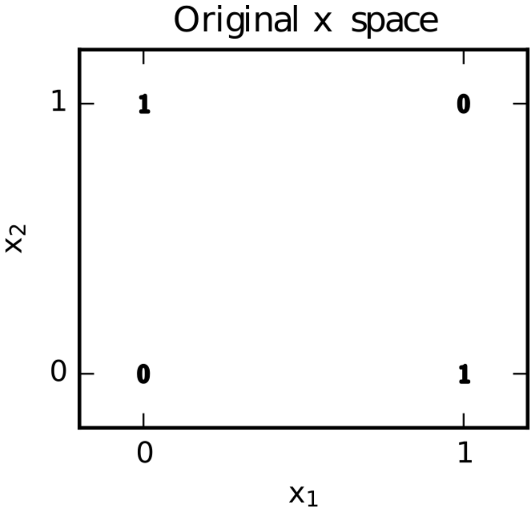


- The perceptron fails at similar problems as a linear SVM
  - **Classical solution:** Feature engineering with Radial Basis Function network $\Rightarrow$ Similar to kernel SVM and good for noisy data
  - **Deep learning solution:** Multilayer networks with nonlinear activations $\Rightarrow$ Good for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

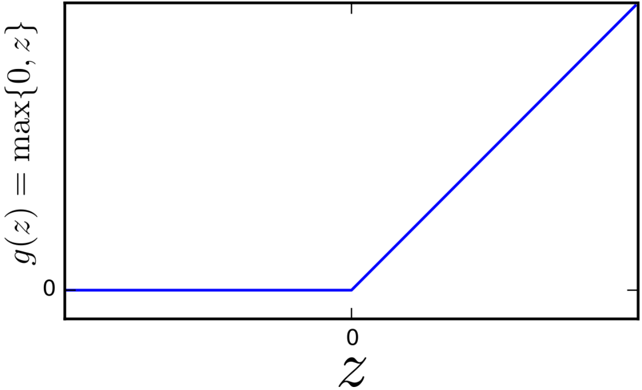
The XOR Problem

- "*Perceptrons*" by Marvin Minsky and Seymour Papert (1969).
- Perceptrons cannot solve the XOR problem.
- Significant decline in interest and funding of neural network research.

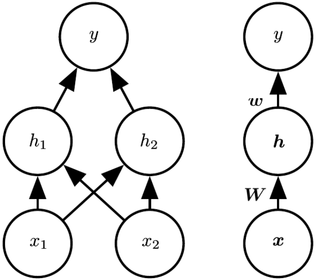
The XOR Problem



Rectified Linear Activation

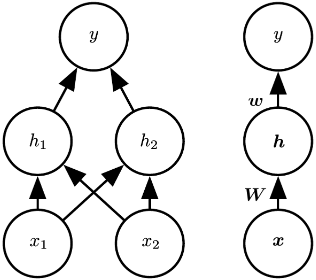


Network Diagrams



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

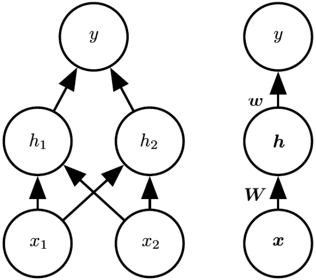
Solving XOR



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

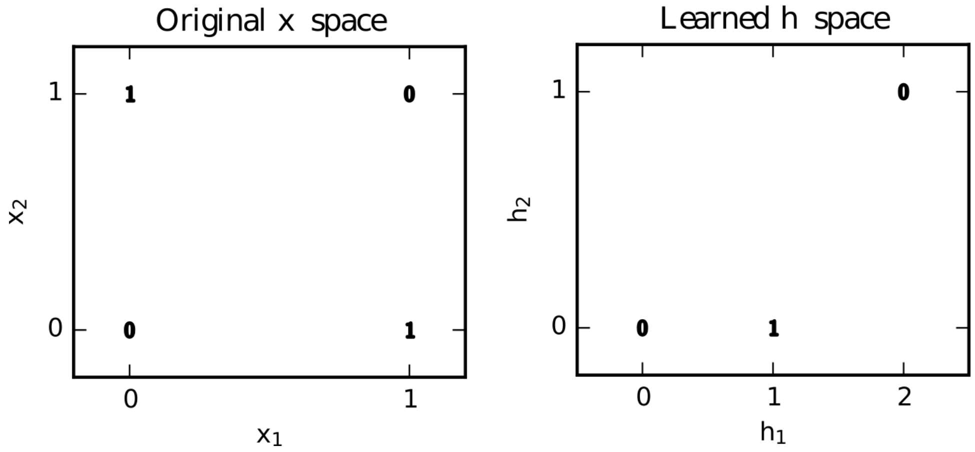
$$X = [\mathbf{x}]_{i=1}^{4} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$
$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$
$$\mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$$
$$\mathbf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$
$$b = 0$$

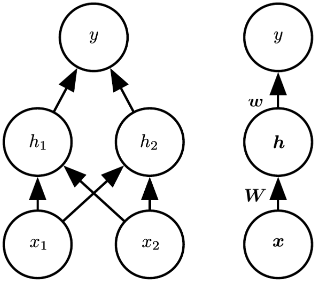
Solving XOR



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

$$H = \max\left(0, \mathbf{W}^T X + \mathbf{c}\right)$$
$$H = \max\left(0, \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 \\ -1 \end{bmatrix}\right)$$
$$H = \max\left(0, \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 1 & 1 & 2 \end{bmatrix} + \begin{bmatrix} 0 \\ -1 \end{bmatrix}\right)$$
$$H = \max\left(0, \begin{bmatrix} 0 & 1 & 1 & 2 \\ -1 & 0 & 0 & 1 \end{bmatrix}\right)$$
$$H = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$


Original x space
1
0
1
0
0
1
0
1
x2
x1
Learned h space
0
0
1
1
0
0
1
2
h2
h1



$$Y = \max\left(0, \mathbf{w}^T H + \mathbf{b}\right)$$

$$Y = \max\left(\left[\begin{array}{cc} 1 & -2 \end{array}\right]\left[\begin{array}{cccc} 0 & 1 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{array}\right] + \left[\begin{array}{c} 0 \\ 0 \end{array}\right]\right)$$

$$Y = \left[\begin{array}{cccc} 0 & 1 & 1 & 0 \end{array}\right]$$

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

Rectified Linear Activation (ReLU)

- Applying this function to the output of a linear transformation yields a nonlinear transformation.
- Very close to linear.
- Very simple nonlinearity (2 pieces – piecewise-linear).
- Sufficient to represent any function if enough hidden units are connected.
- Default activation function recommended for use with most feedforward NNs.

Why ReLU is so effective?

- Strong gradient. Gradient descent can compute large gradients.
- Consistent behavior across its whole domain.
- Historical reasons.

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 $\Phi(v)$ in the output layer can control the nature of the output (e.g., probability value in $[0, 1]$)
- In *multilayer* neural networks, activation functions bring nonlinearity into hidden layers, which increases the complexity of the model.
- Activation functions required for inference may be different from those used in loss functions in training.
  - Perceptron uses sign function $\Phi(v) = \text{sign}(v)$ 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.

Factors

- Nonlinearity.
- Continuously differentiable.
- Range.
- Monotonicity.
- Smooth.
- Approximating identity near the origin.

Summary

Identity Activation

- Identity activation $\Phi(v) = v$ is often used in the output layer, when the outputs are real values.
- 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

Sign Activation

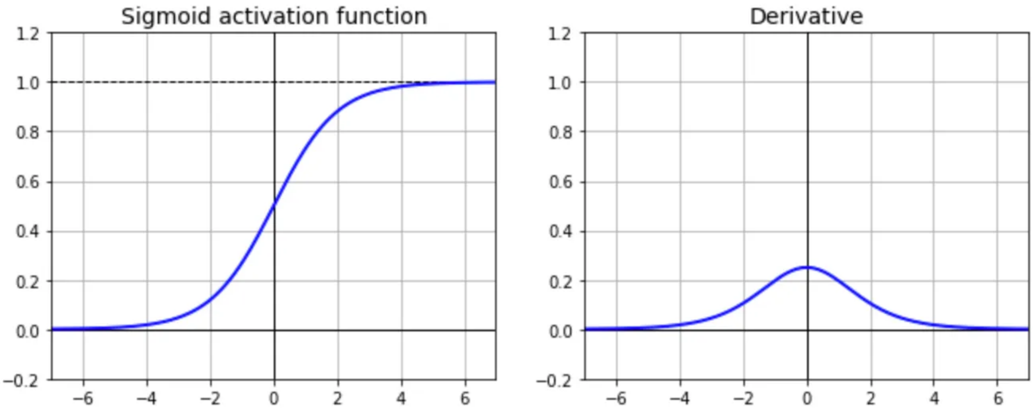
- $\Phi(v) = \begin{cases} +1 & \text{if } v > 0; \\ -1 & \text{if } v < 0. \end{cases}$
- Can be used to map to binary outputs at prediction time.
- Its non-differentiability prevents its use for creating the loss function at training time.
- Eg. while the perceptron uses the sign function for prediction, in training it requires only the linear activation.

Summary

Sigmoid Activation

- Sigmoid activation is defined as $\Phi(v) = 1/(1 + \text{exp}(-v))$.
- For a training pair $(\overline{X}, y)$, one obtains the following prediction in a single-layer network:
$$\hat{y} = 1/(1 + \text{exp}(-\overline{W} \cdot \overline{X}))$$
- Prediction is the *probability* that class label is $+1$.
- Paired with *logarithmic loss*, which $-\text{log}(\hat{y})$ for positive instances and $-\text{log}(1 - \hat{y})$ for negative instances.
  - $\mathcal{L}(\hat{y}, y) = -\left[y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})\right]$
- 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 differentiable. That means we can find the slope of the sigmoid curve at any two points.
- The function is monotonic but the function's derivative is not.

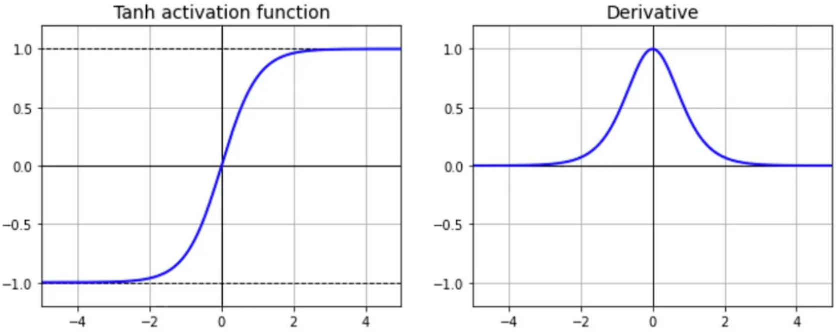
Sigmoid Activation

Drawbacks:

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

Summary

Tanh Activation



- The tanh activation is a scaled and translated version of sigmoid activation.

$$\tanh(v) = \frac{e^{2v} - 1}{e^{2v} + 1} = 2 \cdot \text{sigmoid}(2v) - 1$$

- Often used in hidden layers of multilayer networks

Tanh Activation

Characteristics.

- 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 is not.

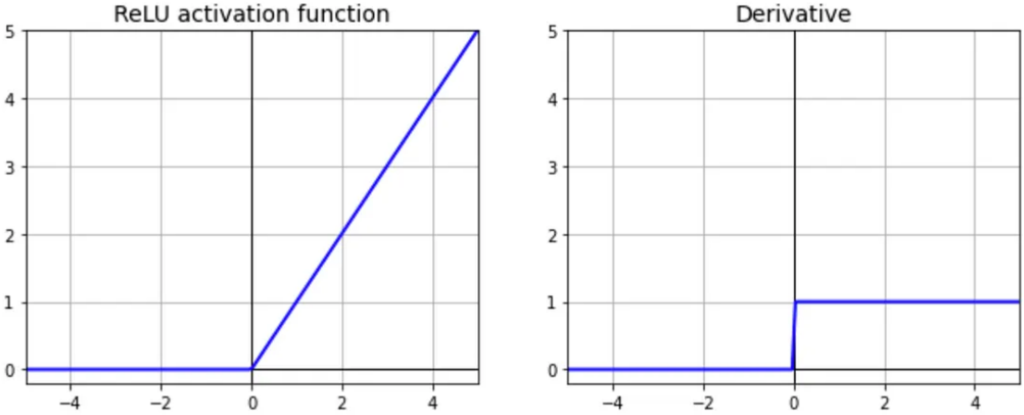
Tanh Activation

Problems:

- Vanishing gradient.
- Computationally expensive.

Summary

Piecewise Linear Activation Functions – ReLU



$$\Phi(v) = \mathsf{max}\{v, 0\}$$

- Piecewise linear activation functions are easier to train than their continuous counterparts.

Piecewise Linear Activation Functions – ReLU

Characteristics:

- Graphically, the ReLU function is composed of two linear pieces to account for non-linearity.
- 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.

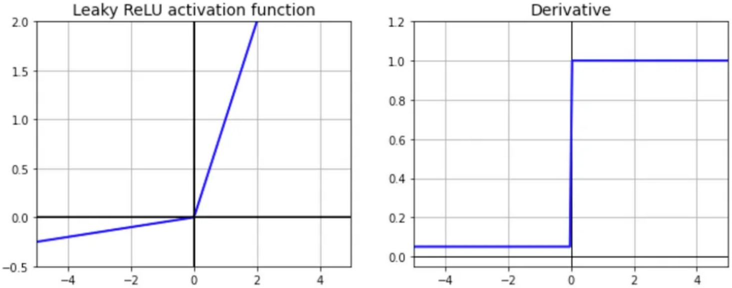
Piecewise Linear Activation Functions – ReLU

Problem:

- Dying ReLU.

Summary

Piecewise Linear Activation Functions – Leaky ReLU

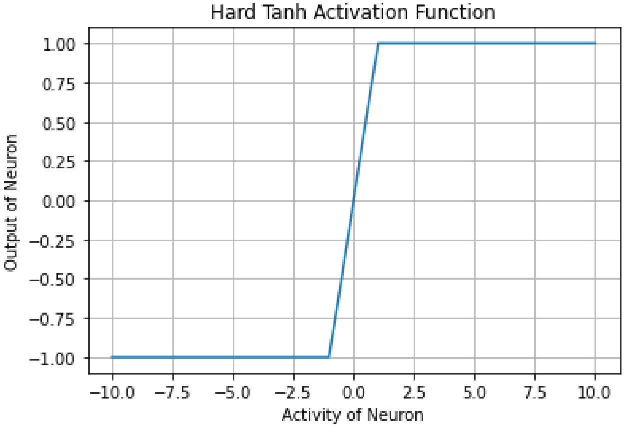


$$\Phi(v) = \mathsf{max}\{\gamma v, v\}$$

Where typically: $\gamma = 0.01$.

Summary

Piecewise Linear Activation Functions – Hard TANH



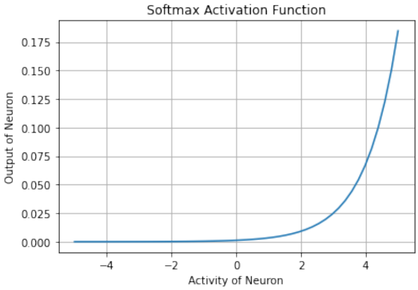
$$\Phi(v) = \max\left\{\min\left[v, 1\right], -1\right\}$$

Summary

Softmax Activation Function

- All activation functions discussed so far map scalars to scalars.
- The softmax activation function maps vectors to vectors.
- Useful in mapping a set of real values to probabilities.
  - Generalization of sigmoid activation, which is used in *multiway* logistic regression.

$$\Phi(\overline{v})_i = \frac{e^{(v_i)}}{\sum_{j=1}^{k} e^{(v_j)}}$$



Derivatives of Activation Functions

- Neural network learning requires gradient descent of the loss.
- Loss is often a function of the output o, which is itself obtained by using the activation function:
$$o = \Phi(v) \tag{1}$$
- Therefore, we often need to compute the partial derivative of o with respect to v during neural network parameter learning.
- Many derivatives are more easily expressed in terms of the output o rather than input v.

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.

$$\begin{aligned}
\overline{h}_1 &= \Phi(W_1^T \overline{x}) = W_1^T \overline{x} \\
\overline{h}_{p+1} &= \Phi(W_{p+1}^T \overline{h}_p) = W_{p+1}^T \overline{h}_p \quad \forall p \in \{1 \dots k-1\} \\
\overline{o} &= \Phi(W_{k+1}^T \overline{h}_k) = W_{k+1}^T \overline{h}_k
\end{aligned}$$

- We can eliminate the hidden variable to get a simple linear relationship:

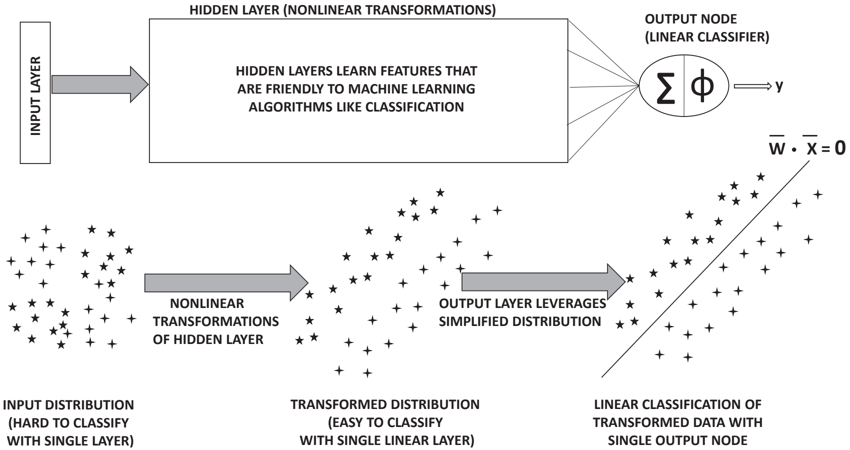
$$\begin{aligned}
\overline{o} &= W_{k+1}^T W_k^T \dots W_1^T \overline{x} \\
&= \underbrace{(W_1 W_2 \dots W_{k+1})^T}_{W_{xo}^T} \overline{x}
\end{aligned}$$

- We get a *single-layer* network with matrix W_{xo}.

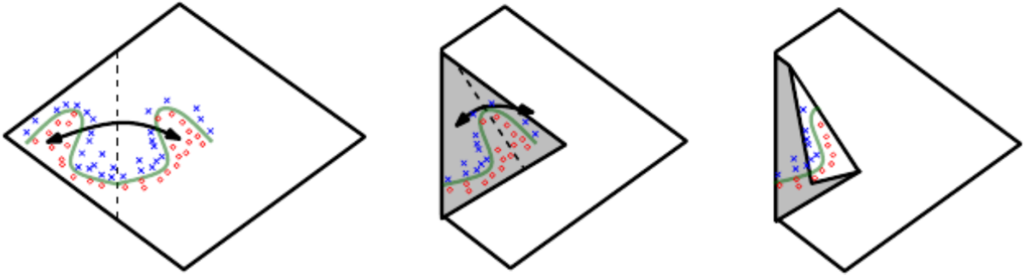
Role of Hidden Layers

- 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.

The Feature Engineering View of Hidden Layers



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



Thank you!

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