Natural Language Processing
Neural Networks

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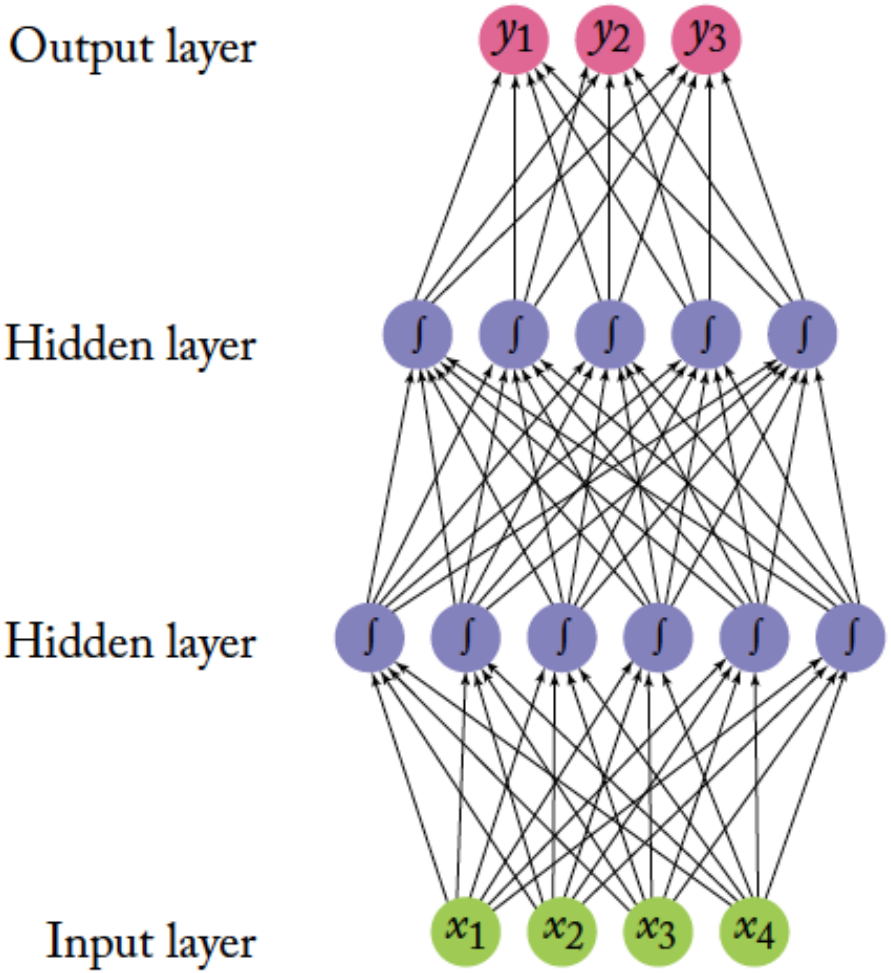
Introduction to Neural Networks

- Very popular machine learning models formed by units called **neurons**.
- A neuron is a computational unit that has scalar inputs and outputs.
- Each input has an associated weight w.
- The neuron multiplies each input by its weight, and then sums them (other functions such as **max** are also possible).
- It applies an activation function g (usually non-linear) to the result, and passes it to its output.
- Multiple layers can be stacked.

Activation Functions

- The nonlinear activation function *g* has a crucial role in the network's ability to represent complex functions.
- Without the nonlinearity in g, the neural network can only represent linear transformations of the input.

Feedforward Network with two Layers



[0]Source:[Goldberg, 2017]

Feedforward Network Neural Networks

- The feedforward network from the picture is a stack of linear models separated by nonlinear functions.
- The values of each row of neurons in the network can be thought of as a vector.
- The input layer is a 4-dimensional vector ($\vec{x}$), and the layer above it is a 6-dimensional vector ($\vec{h}^1$).
- The fully connected layer can be thought of as a linear transformation from 4 dimensions to 6 dimensions.
- A fully connected layer implements a vector-matrix multiplication, $\vec{h} = \vec{x}W$.
- The weight of the connection from the i-th neuron in the input row to the j-th neuron in the output row is $W_{[i,j]}$.
- The values of $\vec{h}$ are transformed by a nonlinear function g that is applied to each value before being passed on as input to the next layer.

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[0] Vectors are assumed to be row vectors and superscript indices correspond to network layers.

Neural Netoworks as Mathematical Functions

- The Multilayer Perceptron (MLP) from the figure is called MLP2 because it has two hidden layers.
- A simpler model would be MLP1, a multilayer perceptron of one hidden layer:

$$NN_{MLP1}(\vec{x}) = g(\vec{x}W^1 + \vec{b}^1)W^2 + \vec{b}^2$$
$$\vec{x} \in \mathcal{R}^{in}, W^1 \in \mathcal{R}^{d_{in} \times d_1}, \vec{b}^1 \in \mathcal{R}^1, W^1 \in \mathcal{R}^{in}, \vec{b}^1 \in \mathcal{R}^{in} \quad (1)$$

- Here W^1 and $\vec{b}^1$ are a matrix and a bias term for the first linear transformation of the input.
- The function g is a nonlinear function that is applied element-wise (also called a nonlinearity or an activation function).
- W^2 and $\vec{b}^2$ are the matrix and bias term for a second linear transform.
- When describing a neural network, one should specify the dimensions of the layers (d_1) and the input (d_{in}).

Neural Netoworks as Mathematical Functions

- MLP2 can be written as the following mathematical function:

$$
\begin{aligned}
NN_{MLP2}(\vec{x}) &= \vec{y} \\
\vec{h}^1 &= g^1(\vec{x}W^1 + \vec{b}^1) \\
\vec{h}^2 &= g^2(\vec{h}^1 W^2 + \vec{b}^2) \\
\vec{y} &= \vec{h}^2 W^3 \\
\vec{y} &= (g^2(g^1(\vec{x}W^1 + \vec{b}^1)W^2 + \vec{b}^2))W^3.
\end{aligned}
\tag{2}
$$

- The matrices and the bias terms that define the linear transformations are the parameters of the network.
- Like in linear models, it is common to refer to the collection of all parameters as Θ.

Representation Power

- [Hornik et al., 1989] and [Cybenko, 1989] showed that a multilayer perceptron of one hidden later (MLP1) is a universal approximator.
- MLP1 can approximate all continuous functions on a closed and bounded subset of $\mathcal{R}^n$.
- This may suggest there is no reason to go beyond MLP1 to more complex architectures.
- The result does not say how easy or hard it is to set the parameters based on training data and a specific learning algorithm.
- It also does not guarantee that a training algorithm will find the correct function generating our training data.
- Finally, it does not state how large the hidden layer should be.

Representation Power

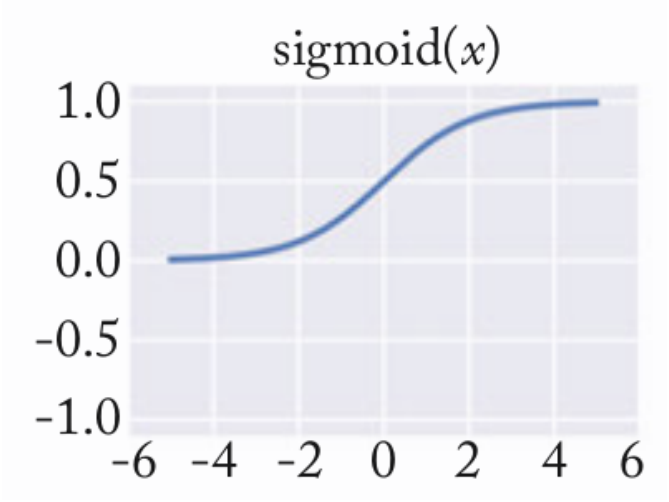
- In practice, we train neural networks on relatively small amounts of data using local search methods.
- We also use hidden layers of relatively modest sizes (up to several thousands).
- The universal approximation theorem does not give any guarantees under these conditions.
- However, there is definitely benefit in trying out more complex architectures than MLP1.
- In many cases, however, MLP1 does indeed provide strong results.

Activation Functions

- The nonlinearity g can take many forms.
- There is currently no good theory as to which nonlinearity to apply in which conditions.
- Choosing the correct nonlinearity for a given task is for the most part an empirical question.

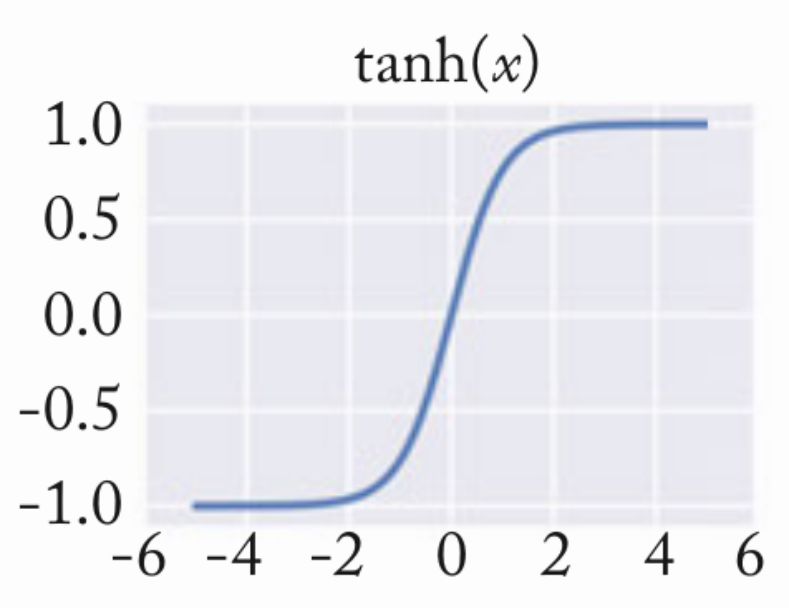
Sigmoid

- The sigmoid activation function $\sigma(x) = \frac{1}{1+e^{-x}}$ is an S-shaped function, transforming each value x into the range $[0, 1]$.
- The sigmoid was the canonical nonlinearity for neural networks since their inception.
- Is currently considered to be deprecated for use in internal layers of neural networks, as the choices listed next prove to work much better empirically.



Hyperbolic tangent (tanh)

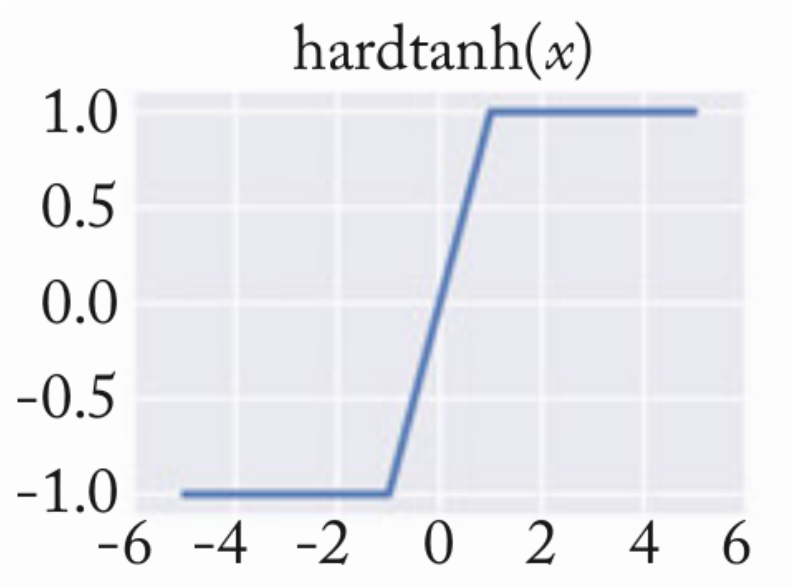
- The hyperbolic tangent $\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$ activation function is an S-shaped function, transforming the values x into the range$[-1, 1]$.



Hard tanh

- The hard-tanh activation function is an approximation of the tanh function which is faster to compute and to find derivatives thereof:

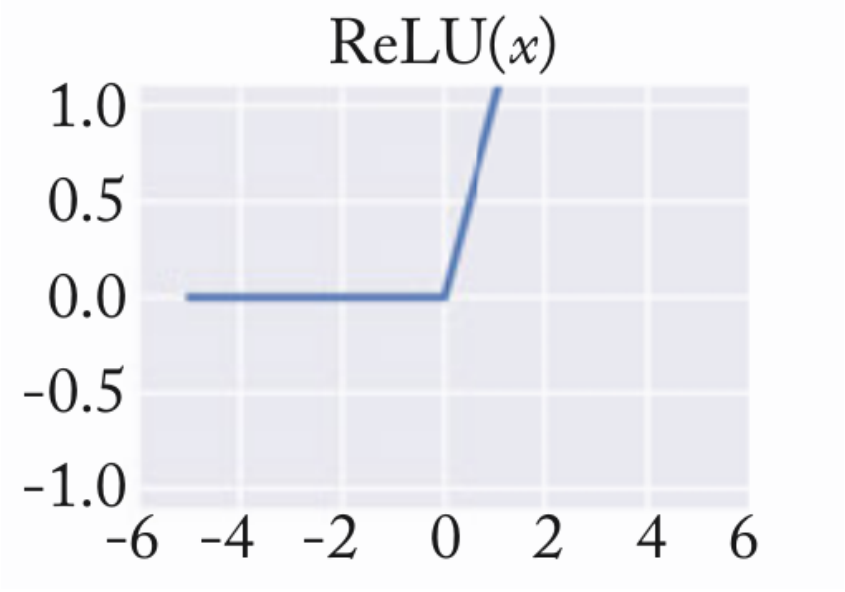
$$\text{hardtanh}(x) = \left\{ \begin{array}{ll} -1 & x < -1 \\ 1 & x > 1 \\ x & \text{otherwise.} \end{array} \right\}$$



ReLU

- The rectifier activation function [Glorot et al., 2011], also known as the recti fied linear unit is a very simple activation function.
- It is easy to work with and was shown many times to produce excellent results.
- The ReLU unit clips each value $x < 0$ at 0.

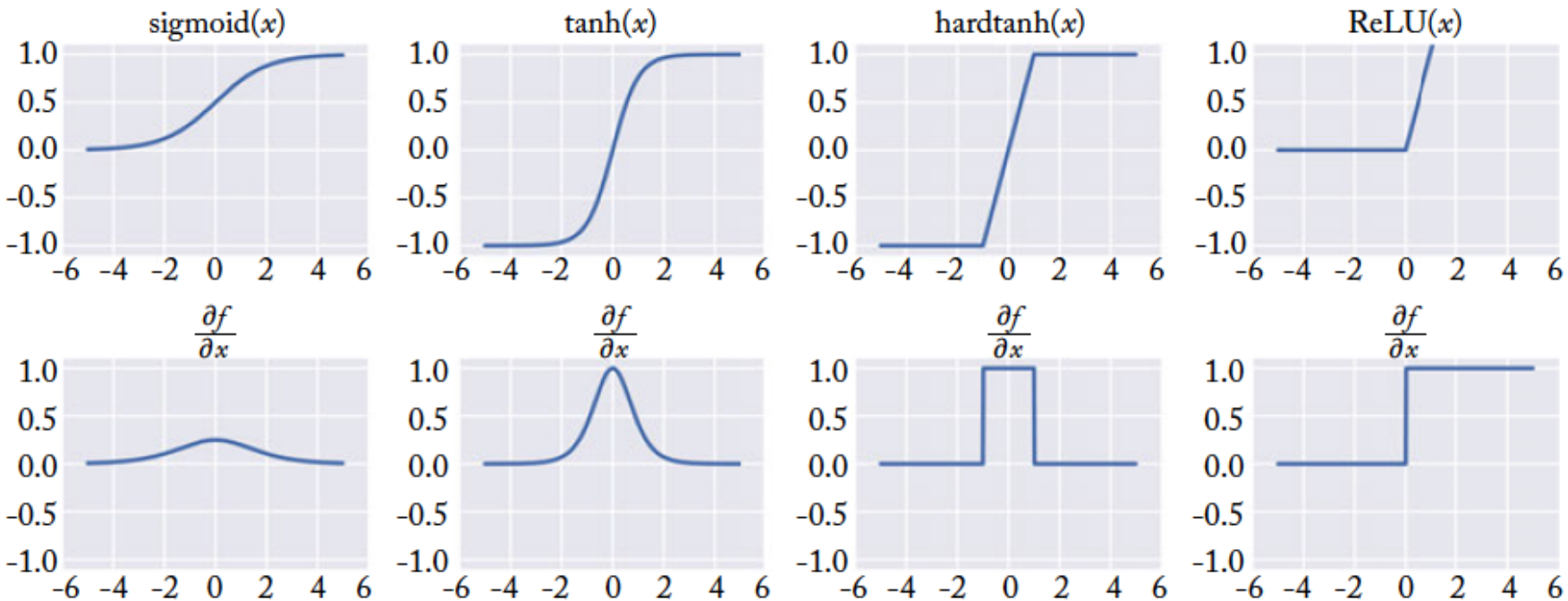
$$\text{ReLU}(x) = \max(0, x)$$



- It performs well for many tasks, especially when combined with the dropout regularization technique (to be explained later).

Activation Functions

- As a rule of thumb, both ReLU and tanh units work well, and significantly outperform the sigmoid.
- You may want to experiment with both tanh and ReLU activations, as each one may perform better in different settings.
- The figure from below shows the shapes of the different activations functions, together with the shapes of their derivatives.

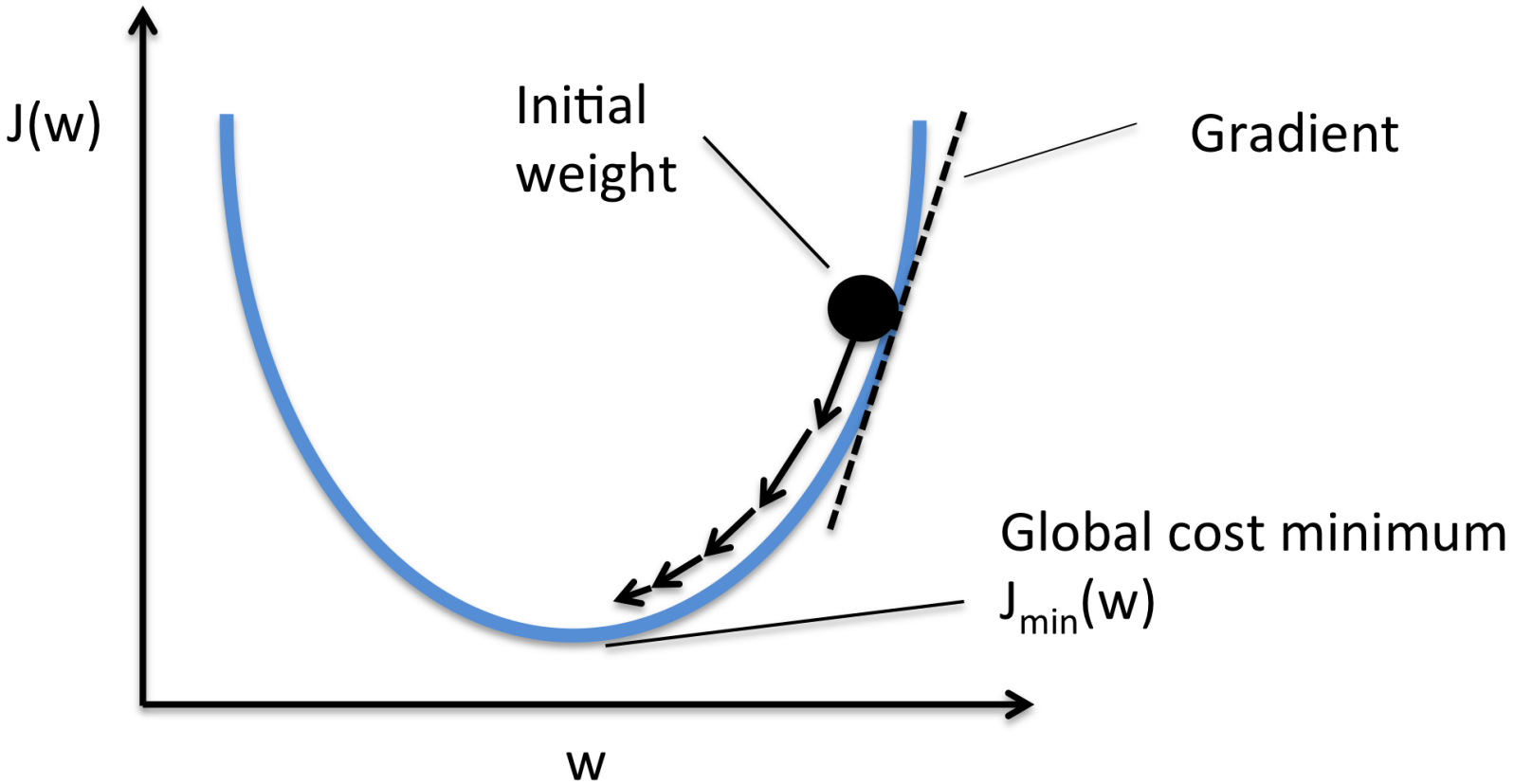


[0]Source:[Goldberg, 2017]

Training

- When training a parameterized function (e.g., a linear model, a neural network) one defines a loss function $L(\hat{y}, y)$, stating the loss of predicting $\hat{y}$ when the true output is y.
- The training objective is then to minimize the loss across the different training examples.
- Functions are trained using gradient-based methods.
- They work by repeatedly computing an estimate of the loss L over the training set.
- They compute gradients of the parameters with respect to the loss estimate, and moving the parameters in the opposite directions of the gradient.
- Different optimization methods differ in how the error estimate is computed, and how moving in the opposite direction of the gradient is defined.

Gradient Descent



[0]Source: https://sebastianraschka.com/images/faq/closed-form-vs-gd/ball.png

Gradient Descent

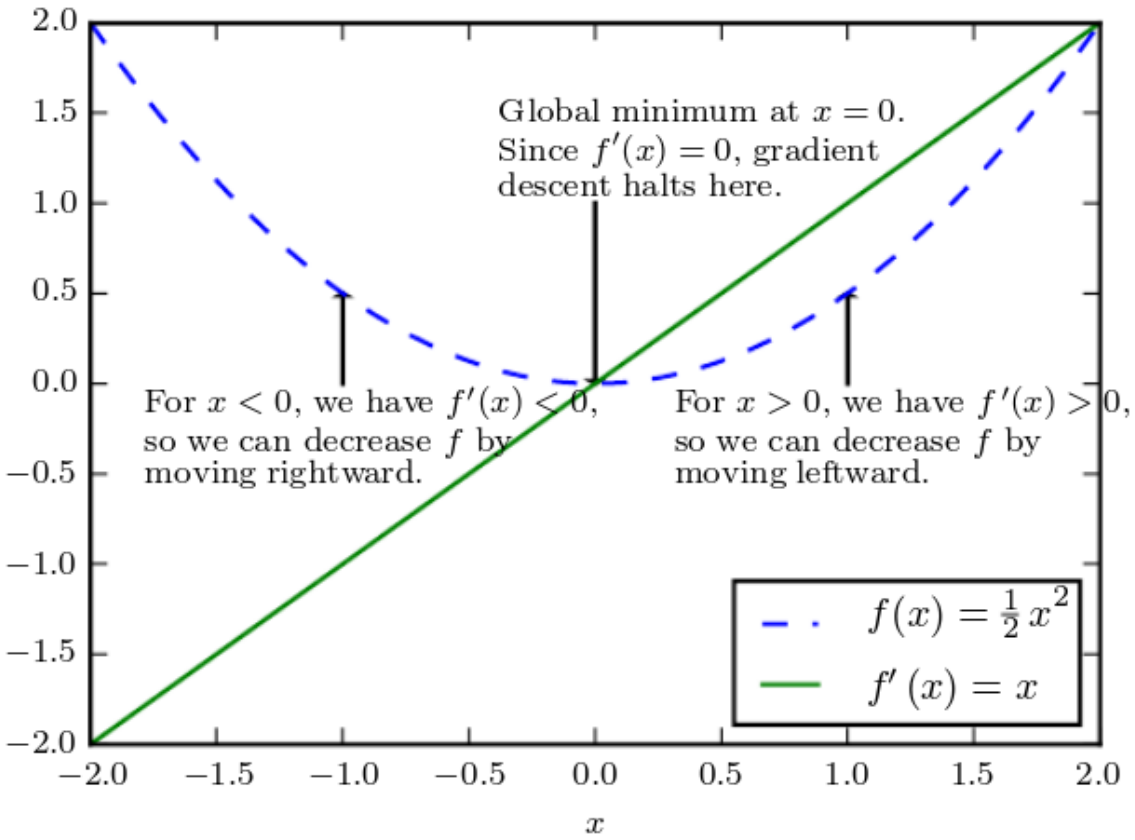


Figure 4.1: Gradient descent. An illustration of how the gradient descent algorithm uses the derivatives of a function to follow the function downhill to a minimum.

[0][Goodfellow et al., 2016]

Online Stochastic Gradient Descent

- All the parameters are initialized with random values w.
- For each training example (x, y) we calculate the loss L with current values of w.
- Then we update the parameters with the following rule until convergence:
- $w_i \leftarrow w_i - \eta \frac{\partial L}{w_i}(x, y)$ (for all parameters w_i)

Algorithm 2.1 Online stochastic gradient descent training.

Input:
- Function $f(\boldsymbol{x}; \Theta)$ parameterized with parameters Θ.
- Training set of inputs $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}$ and desired outputs $\boldsymbol{y_1}, \ldots, \boldsymbol{y_n}$.
- Loss function L.

1: **while** stopping criteria not met **do**
2: Sample a training example $\boldsymbol{x_i}, \boldsymbol{y_i}$
3: Compute the loss $L(f(\boldsymbol{x_i}; \Theta), \boldsymbol{y_i})$
4: $\hat{\boldsymbol{g}} \leftarrow$ gradients of $L(f(\boldsymbol{x_i}; \Theta), \boldsymbol{y_i})$ w.r.t Θ
5: $\Theta \leftarrow \Theta - \eta_t \hat{\boldsymbol{g}}$
6: **return** Θ

[0]Source:[Goldberg, 2017]

Online Stochastic Gradient Descent

- The learning rate can either be fixed throughout the training process, or decay as a function of the time step t.
- The error calculated in line 3 is based on a single training example, and is thus just a rough estimate of the corpus-wide loss L that we are aiming to minimize.
- The noise in the loss computation may result in inaccurate gradients (single examples may provide noisy information).

Mini-batch Stochastic Gradient Descent

- A common way of reducing this noise is to estimate the error and the gradients based on a sample of *m* examples.
- This gives rise to the minibatch SGD algorithm

Algorithm 2.2 Minibatch stochastic gradient descent training.

Input:
- Function $f(\boldsymbol{x};\Theta)$ parameterized with parameters Θ.
- Training set of inputs $\boldsymbol{x_1},\ldots,\boldsymbol{x_n}$ and desired outputs $\boldsymbol{y_1},\ldots,\boldsymbol{y_n}$.
- Loss function L.

1: **while** stopping criteria not met **do**
2: Sample a minibatch of m examples $\{(\boldsymbol{x_1},\boldsymbol{y_1}),\ldots,(\boldsymbol{x_m},\boldsymbol{y_m})\}$
3: $\hat{\boldsymbol{g}} \leftarrow 0$
4: **for** $i = 1$ to m **do**
5: Compute the loss $L(f(\boldsymbol{x_i};\Theta),\boldsymbol{y_i})$
6: $\hat{\boldsymbol{g}} \leftarrow \hat{\boldsymbol{g}} +$ gradients of $\frac{1}{m}L(f(\boldsymbol{x_i};\Theta),\boldsymbol{y_i})$ w.r.t Θ
7: $\Theta \leftarrow \Theta - \eta_t\hat{\boldsymbol{g}}$
8: **return** Θ

- Higher values of *m* provide better estimates of the corpus-wide gradients, while smaller values allow more updates and in turn faster convergence.
- For modest sizes of *m* , some computing architectures (i.e., GPUs) allow an efficient parallel implementation of the computation in lines 3-6.

[0]Source:[Goldberg, 2017]

Loss Functions

- Hinge (or SVM loss): for binary classification problems, the classifier's output is a single scalar $\tilde{y}$ and the intended output y is in $\{+1, -1\}$. The classification rule is $\hat{y} = sign(\tilde{y})$, and a classification is considered correct if $y \cdot \tilde{y} > 0$.

$$L_{\text{hinge(binary)}}(\tilde{y}, y) = \max(0, 1 - y \cdot \tilde{y})$$

- Binary cross entropy (or logistic loss): is used in binary classification with conditional probability outputs. The classifier's output $\tilde{y}$ is transformed using the sigmoid function to the range $[0, 1]$, and is interpreted as the conditional probability $P(y = 1|x)$.

$$L_{\text{logistic}}(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

Loss Functions

- Categorical cross-entropy loss: is used when a probabilistic interpretation of multi-class scores is desired. It measures the dissimilarity between the true label distribution y and the predicted label distribution $\tilde{y}$.

$$L_{\text{cross-entropy}}(\hat{y}, y) = -\sum_i y_{[i]} \log(\hat{y}_{[i]})$$

- The predicted label distribution of the categorical cross-entropy loss ($\hat{y}$) is obtained by applying the softmax function the last layer of the network $\tilde{y}$:

$$\hat{y}_{[i]} = \text{softmax}(\tilde{y})_{[i]} = \frac{e^{\tilde{y}_{[i]}}}{\sum_j e^{\tilde{y}_{[j]}}}$$

- The softmax function squashes the k-dimensional output to values in the range (0,1) with all entries adding up to 1. Hence, $\hat{y}_{[i]} = P(y = i|x)$ represent the class membership conditional distribution.

Backpropagation

- Backpropagation is an efficient technique for evaluating the gradient of a loss function L for a feed-forward neural network with respect to all its parameters [Bishop, 2006]. [1]
- Those parameters are: $W^1, \vec{b}^1, \ldots, W^m, \vec{b}^m$, for a network of m layers.
- Recall that superscripts are used to denote layer indexes (not exponentiations).
- For simplicity, we will assume that L is calculated over a single example.
- In a general feed-forward network, each unit computes a weighted sum of its inputs in the form:

$$\vec{h}^l_{[j]} = \left(\sum_i W^l_{[i,j]} \times \vec{z}^{(l-1)}_{[i]} \right) + \vec{b}^l_{[j]} \tag{3}$$

- The variable $\vec{z}^{(l-1)}_{[i]}$ is an input that sends a connection to unit $\vec{h}^l_{[j]}$, $W^l_{[i,j]}$ is the weight associated with that connection, and l is the layer index.
- The biases vectors $\vec{b}_{[j]}$ can be excluded from (eq.3) and included to the weight matrix $W^l_{[i,j]}$ by introducing an extra unit, or input, with activation fixed at +1.

[1] The following slides on backpropagation are based on [Bishop, 2006], we adapted the notation to be consistent with [Goldberg, 2017].

Backpropagation

- The inputs at layer l, $\vec{z}_{[i]}^{(l-1)}$ are the result of applying the activation function g to units from the previous layer:

$$\vec{z}_{[j]}^{l} = g(\vec{h}_{[j]}^{l}) \tag{4}$$

- For the input layer ($l = 0$), $\vec{z}$ corresponds to the input vector $\vec{z} = \vec{x}$

$$\vec{z}_{[j]}^{0} = \vec{x}_{[j]} \tag{5}$$

- For each instance in the training set, we supply the corresponding input vector $\vec{x}$ to the network.
- Next we calculate the activations of all of the hidden and output units in the network by successive application of (eq.3) and (eq.4).
- This process is often called forward propagation because it can be regarded as a forward flow of information through the network.

Backpropagation

- Now consider the evaluation of the derivative of L with respect to a weight $W^l_{[i,j]}$.
- Assuming that the loss L is calculated over a single example, we can note that L depends on the weight $W^l_{[i,j]}$ only via the summed input $\vec{h}^l_{[j]}$.
- We can therefore apply the chain rule for partial derivatives to give

$$\frac{\partial L}{\partial W^l_{[i,j]}} = \frac{\partial L}{\partial \vec{h}^l_{[j]}} \times \frac{\partial \vec{h}^l_{[j]}}{\partial W^l_{[i,j]}} \tag{6}$$

Backpropagation

- We now introduce a useful notation:

$$\vec{\delta}^{l}_{[j]} \equiv \frac{\partial L}{\partial \vec{h}^{l}_{[j]}} \tag{7}$$

- Using (3), we can write

$$\frac{\partial \vec{h}^{l}_{[j]}}{\partial W^{l}_{[i,j]}} = \vec{z}^{(l-1)}_{[i]} \tag{8}$$

- Substituting (7) and (8) into (6), we then obtain

$$\frac{\partial L}{\partial W^{l}_{[i,j]}} = \vec{\delta}^{l}_{[j]} \times \vec{z}^{(l-1)}_{[i]} \tag{9}$$

Backpropagation

- Equation (9) tells us that the required derivative is obtained simply by multiplying the value of $\vec{\delta}_{[j]}^{l}$ by the value of $\vec{z}_{[i]}^{(l-1)}$.
- Thus, in order to evaluate the derivatives, we need only to calculate the value of $\vec{\delta}_{[j]}^{l}$ for each hidden and output unit in the network, and then apply (9).
- Calculating $\vec{\delta}_{[j]}^{m}$ for output units ($l = m$), is usually straightforward, since activation units $\vec{h}_{[j]}^{m}$ are directly observed in the loss expression.
- The same applies for shallow linear models.

Backpropagation

- To evaluate the $\vec{\delta}^{l}_{[j]}$ for hidden units, we again make use of the chain rule for partial derivatives:

$$\vec{\delta}^{l}_{[j]} \equiv \frac{\partial L}{\partial \vec{h}^{l}_{[j]}} = \sum_{k} \left(\frac{\partial L}{\partial \vec{h}^{l+1}_{[k]}} \times \frac{\partial \vec{h}^{l+1}_{[k]}}{\partial \vec{h}^{l}_{[j]}} \right) \tag{10}$$

- The sum runs over all units $\vec{h}^{l+1}_{[k]}$ to which unit $\vec{h}^{l}_{[j]}$ sends connections.
- We assume that connections go only to consecutive layers in the network (from layer l to layer $(l+1)$).
- The units $\vec{h}^{l+1}_{[k]}$ could include other hidden units and/or output units.
- If we now substitute the definition of $\vec{\delta}^{l}_{[j]}$ given by (eq.7) into (eq.10), we get

$$\vec{\delta}^{l}_{[j]} \equiv \frac{\partial L}{\partial \vec{h}^{l}_{[j]}} = \sum_{k} \left(\vec{\delta}^{(l+1)}_{[k]} \times \frac{\partial \vec{h}^{l+1}_{[k]}}{\partial \vec{h}^{l}_{[j]}} \right) \tag{11}$$

Backpropagation

- Now, for expression $\vec{h}^{l+1}_{[k]}$ we can go to its definition (eq.3):

$$\vec{h}^{(l+1)}_{[k]} = \left(\sum_i W^{l+1}_{[i,k]} \times \vec{z}^{l}_{[i]} \right) + \vec{b}^{(l+1)}_{[k]}$$

- Now, we replace (eq.4) ($\vec{z}^{l}_{[i]} = g(\vec{h}^{l}_{[i]})$) into previous equation and we obtain:

$$\vec{h}^{(l+1)}_{[k]} = \left(\sum_i W^{l+1}_{[i,k]} \times g(\vec{h}^{l}_{[i]}) \right) + \vec{b}^{(l+1)}_{[k]}$$

- Now when calculating $\frac{\partial \vec{h}^{l+1}_{[k]}}{\partial \vec{h}^{l}_{[j]}}$ all the terms in the summation where $i \neq j$ get canceled out.
- Hence:

$$\frac{\partial \vec{h}^{l+1}_{[k]}}{\partial \vec{h}^{l}_{[j]}} = W^{l+1}_{[j,k]} \times g'(\vec{h}^{l}_{[j]}) \tag{12}$$

Backpropagation

- Now, if we substitute (eq.12) into (eq.11)

$$\vec{\delta}^{l}_{[j]} \equiv \frac{\partial L}{\partial \vec{h}^{l}_{[j]}} = \sum_{k} \left(\vec{\delta}^{(l+1)}_{[k]} \times W^{l+1}_{[j,k]} \times g'(\vec{h}^{l}_{[j]}) \right) \tag{13}$$

- Since $g'(\vec{h}^{l}_{[j]})$ doesn't depend on k we can obtain the following backpropagation formula:

$$\vec{\delta}^{l}_{[j]} = g'(\vec{h}^{l}_{[j]}) \times \sum_{k} \left(\vec{\delta}^{(l+1)}_{[k]} \times W^{l+1}_{[j,k]} \right) \tag{14}$$

- Which tells us that the value of δ for a particular hidden unit can be obtained by propagating the δ's backwards from units higher up in the network.
[Bishop, 2006].

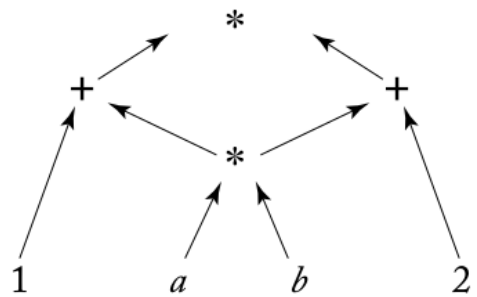
Backpropagation

The backpropagation procedure can be summarized as follows.

1. Apply an input vector $\vec{x}$ to the network and forward propagate through the network using (eq.3) and (eq.4) to find the activations of all the hidden and output units.
2. Evaluate the $\vec{\delta}^{m}_{[j]}$ for all the output units (recall that the derivatives involved here are easy to calculate).
3. Backpropagate the $\vec{\delta}^{(l+1)}_{[k]}$ using (eq.14) to obtain $\vec{\delta}^{l}_{[j]}$ for each hidden unit in the network. We go from higher to lower layers in the network.
4. Use (eq.9) ($\frac{\partial L}{\partial w^{l}_{[i,j]}} = \vec{\delta}^{l}_{[j]} \times \vec{z}^{(l-1)}_{[i]}$) to evaluate the required derivatives.

The Computation Graph Abstraction

- One can compute the gradients of the various parameters of a network by hand and implement them in code.
- This procedure is cumbersome and error prone.
- For most purposes, it is preferable to use automatic tools for gradient computation [Bengio, 2012].
- A computation graph is a representation of an arbitrary mathematical computation (e.g., a neural network) as a graph.
- Consider for example a graph for the computation of $(a * b + 1) * (a * b + 2)$:



- The computation of $a * b$ is shared.
- The graph structure defines the order of the computation in terms of the dependencies between the different components.

The Computation Graph Abstraction

- Te computation graph abstraction allows us to:
  1. Easily construct arbitrary networks.
  2. Evaluate their predictions for given inputs (forward pass)

Algorithm 5.3 Computation graph forward pass.

1: **for** i = 1 to N **do**
2: Let $a_1, \ldots, a_m = \pi^{-1}(i)$
3: $v(i) \leftarrow f_i(v(a_1), \ldots, v(a_m))$

  3. Compute gradients for their parameters with respect to arbitrary scalar losses (backward pass or backpropagation).

Algorithm 5.4 Computation graph backward pass (backpropagation).

1: $d(N) \leftarrow 1$ ▷ $\frac{\partial N}{\partial N} = 1$
2: **for** i = N-1 to 1 **do**
3: $d(i) \leftarrow \sum_{j \in \pi(i)} d(j) \cdot \frac{\partial f_j}{\partial i}$ ▷ $\frac{\partial N}{\partial i} = \sum_{j \in \pi(i)} \frac{\partial N}{\partial j} \frac{\partial j}{\partial i}$

- The backpropagation algorithm (backward pass) is essentially following the chain-rule of differentiation[2].

[2] A comprehensive tutorial on the backpropagation algorithm over the computational graph abstraction:
https://colah.github.io/posts/2015-08-Backprop/

Train, Test, and Validation Sets

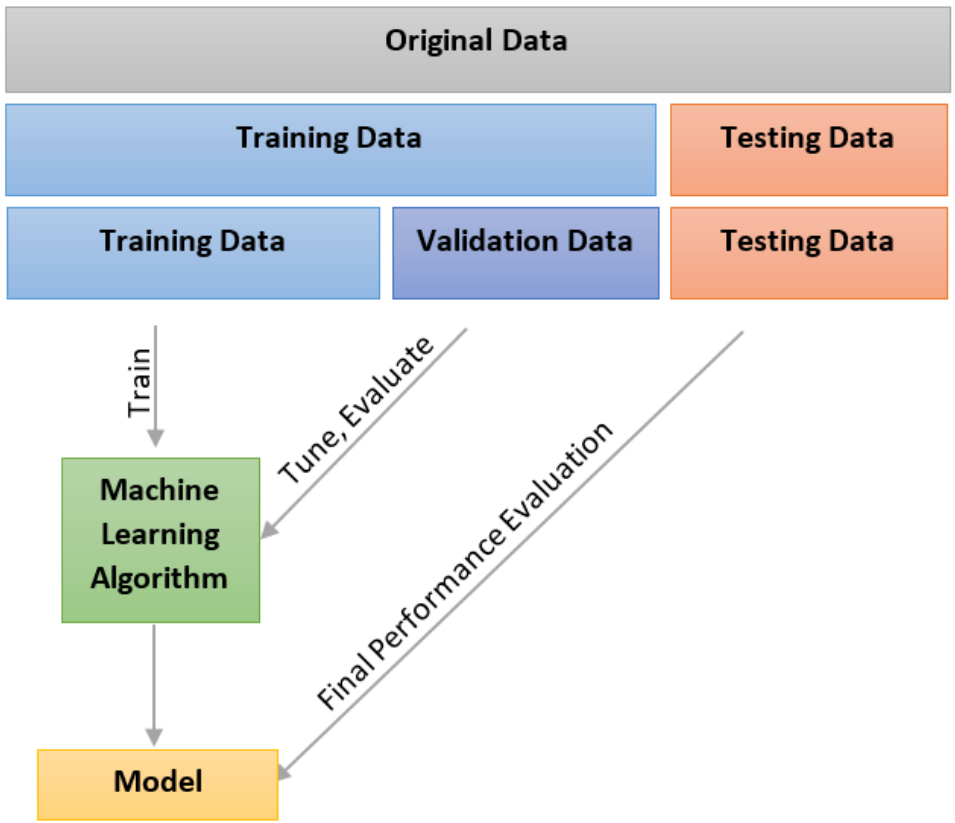
- Neural networks are prone to overfit the data.
- Hence, performance on training data can be misleading.
- Held-out set: split training set into training and testing subsets (80% and 20% splits). Train on training and compute accuracy on testing.
- Problem: in practice you often train several models, compare their quality, and select the best one.
- Selecting the best model according to the held-out set's accuracy will result in an overly optimistic estimate of the model's quality.
- You don't know if the chosen settings of the final classifier are good in general, or are just good for the particular examples in the held-out sets.

Train, Test, and Validation Sets

- The accepted methodology is to use a three-way split of the data into train, validation (also called development), and test sets [3].
- This gives you two held-out sets: a validation set (also called development set), and a test set.
- All the experiments, tweaks, error analysis, and model selection should be performed based on the validation set.
- Then, a single run of the final model over the test set will give a good estimate of its expected quality on unseen examples.
- It is important to keep the test set as pristine as possible, running as few experiments as possible on it.
- Some even advocate that you should not even look at the examples in the test set, so as to not bias the way you design your model.

[3] An alternative approach is cross-validation, but it doesn't scale well for training deep neural networks.

Train, Test, and Validation Sets



[3]source: https://www.codeproject.com/KB/AI/1146582/validation.PNG

Deep Learning Frameworks

Several software packages implement the computation-graph model. All these packages support all the essential components (node types) for defining a wide range of neural network architectures.

- TensorFlow (`https://www.tensorflow.org/`): an open source software library for numerical computation using data-flow graphs originally developed by the Google Brain Team.
- Keras: High-level neural network API that runs on top of Tensorflow as well as other backends (`https://keras.io/`).
- PyTorch: open source machine learning library for Python, based on Torch, developed by Facebook's artificial-intelligence research group. It supports dynamic graph construction, a different computation graph is created from scratch for each training sample. (`https://pytorch.org/`)

Questions?

Thanks for your Attention!

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