Natural Language Processing
Neural Networks

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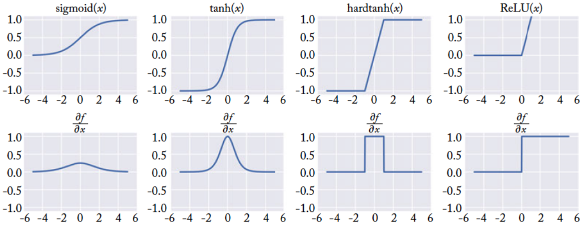
Introduction to Neural Networks

- 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.

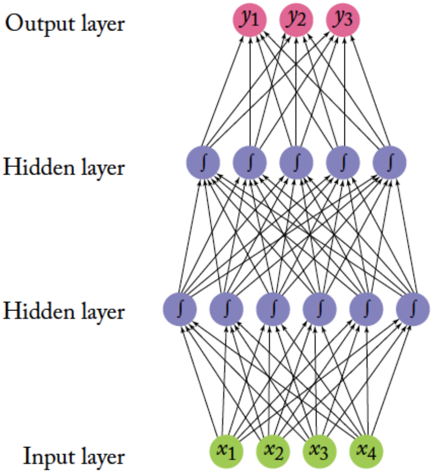
Activation Functions

- 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.



[0] Source:[Goldberg, 2016]

Feedforward Network with two Layers



[0] Source:[Goldberg, 2016]

Brief Introduction to 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.

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

Brief Introduction to Neural Networks

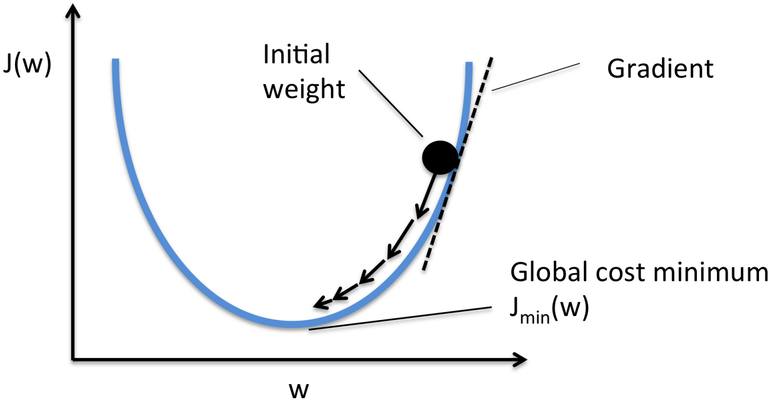
- The Multilayer Perceptron (MLP) from the figure can be written as the following mathematical function:

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

Network Training

- When training 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.
- Networks 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`

Online Stochastic Gradient Descent

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

- 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).

[0] Source:[Goldberg, 2016]

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: $\hat{g} \leftarrow 0$
4: **for** $i = 1$ to m **do**
5: Compute the loss $L(f(\boldsymbol{x_i}; \Theta), \boldsymbol{y_i})$
6: $\hat{g} \leftarrow \hat{g} +$ gradients of $\frac{1}{m} L(f(\boldsymbol{x_i}; \Theta), \boldsymbol{y_i})$ w.r.t Θ
7: $\Theta \leftarrow \Theta - \eta_t \hat{g}$
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, 2016]

Some 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 $P(y = 1|x)$.

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

Some 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 $\tilde{y}$.

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

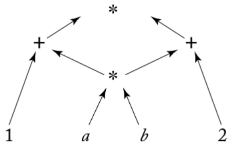
- The predicted label distribution of the categorical cross-entropy loss ($\hat{y}$) is obtained by applying the softmax function the last layer of the network $\tilde{y}$:

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

- 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.

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 $a_1, \dots, a_m = \pi^{-1}(i)$
3: $v(i) \leftarrow f_i(v(a_1), \dots, v(a_m))$

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

- The backpropagation algorithm (backward pass) is essentially following the chain-rule of differentiation[1].

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

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!

References I

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