Natural Language Processing
Linear Models and Neural Networks

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Supervised Learning

- The essence of supervised machine learning is the creation of mechanisms that can look at examples and produce generalizations. [Goldberg, 2017]
- We design an algorithm whose input is a set of labeled examples, and its output is a function (or a program) that receives an instance and produces the desired label.
- Example: if the task is to distinguish from spam and not-spam email, the labeled examples are emails labeled as spam and emails labeled as not-spam.
- It is expected that the resulting function will produce correct label predictions also for instances it has not seen during training.
- This approach differs from designing an algorithm to perform the task (e.g., manually designed rule-based systems).

Parameterized Functions

- Searching over the set of all possible functions is a very hard (and rather ill-defined) problem. [Goldberg, 2017]
- We often restrict ourselves to search over specific families of functions.
- Example: the space of all linear functions with d_{in} inputs and d_{out} outputs,
- Such families of functions are called **hypothesis classes**.
- By restricting ourselves to a specific hypothesis class, we are injecting the learner with **inductive bias**.
- Inductive bias: a set of assumptions about the form of the desired solution.
- Some hypothesis classes facilitate efficient procedures for searching for the solution. [Goldberg, 2017]

Linear Models

- One common hypothesis class is that of high-dimensional linear function:

$$
\begin{aligned}
f(x) = \vec{x} \cdot W + \vec{b} \\
\vec{x} \in \mathcal{R}^{d_{in}} \quad W \in \mathcal{R}^{d_{in} \times d_{out}} \quad \vec{b} \in \mathcal{R}^{d_{out}}
\end{aligned}
\tag{1}
$$

- The vector $\vec{x}$ is the input to the function.
- The matrix W and the vector $\vec{b}$ are the parameters.
- The goal of the learner is to set the values of the parameters W and $\vec{b}$ such that the function behaves as intended on a collection of input values $\vec{x}_{1:k} = \vec{x}_1, \ldots, \vec{x}_k$ and the corresponding desired outputs $\vec{y}_{1:k} = \vec{y}_1, \ldots, \vec{y}_k$
- The task of searching over the space of functions is thus reduced to one of searching over the space of parameters. [Goldberg, 2017]

Example: Language Detection

- Consider the task of distinguishing documents written in English from documents written in German.
- This is a binary classifcation problem

$$f(x) = \vec{x} \cdot w + b \tag{2}$$

$d_{out} = 1$, w is a vector, and b is a scalar.

- The range of the linear function in is $[-\infty, \infty]$.
- In order to use it for binary classification, it is common to pass the output of $f(x)$ through the *sign* function, mapping negative values to -1 (the negative class) and non-negative values to +1 (the positive class).

Example: Language Detection

- Letter frequencies make for quite good predictors (features) for this task.
- Even more informative are counts of letter bigrams , i.e., pairs of consecutive letters.
- We assume we have an alphabet of 28 letters (a–z, space, and a special symbol for all other characters including digits, punctuations, etc.)
- Documents are represented as 28×28 dimensional vectors $\vec{x} \in \mathcal{R}^{784}$.
- Each entry $\vec{x}_{[i]}$ represents a count of a particular letter combination in the document, normalized by the document's length.

Example: Language Detection

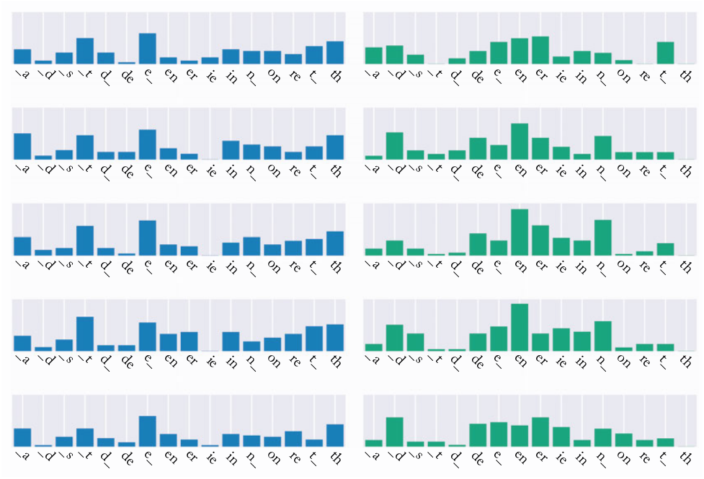


Figure: Character-bigram histograms for documents in English (left, blue) and German(right,green). Underscores denote spaces.

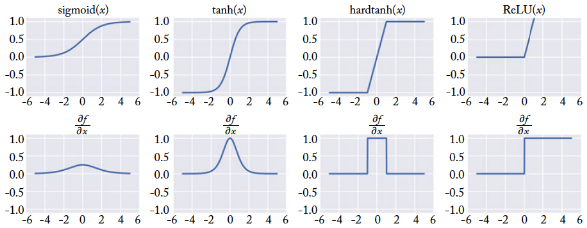
[0]Source:[Goldberg, 2016]

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.

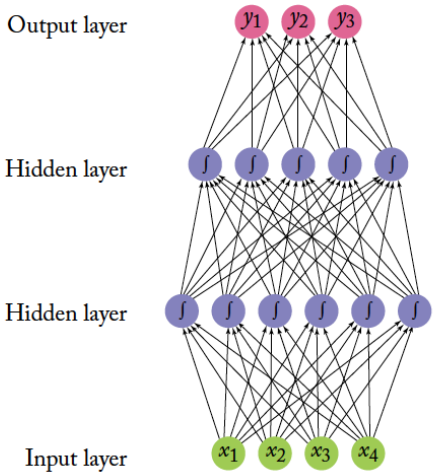
Activation Functions

- 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

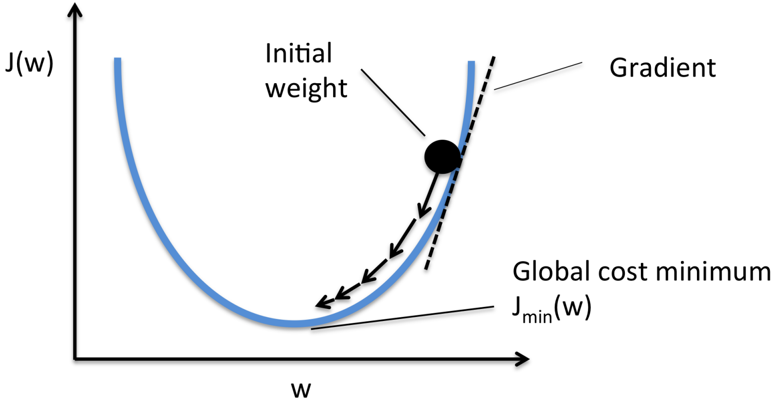
- The Multilayer Perceptron (MLP) from the figure can be written as the following mathematical function:

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

Network Training

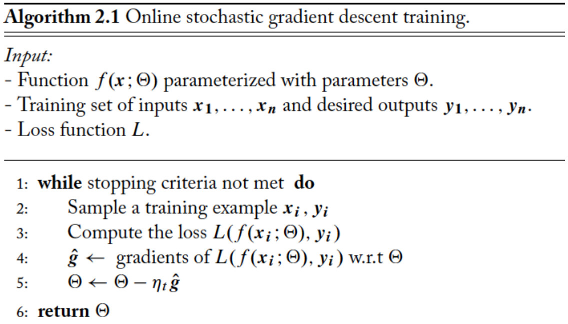
- When training a neural network one defines a loss function $L(\hat{y}, y)$, stating the loss of predicting $\hat{y}$ when the true output is y.
- The training objective is then to minimize the loss across the different training examples.
- Networks are trained using gradient-based methods.
- They work 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.

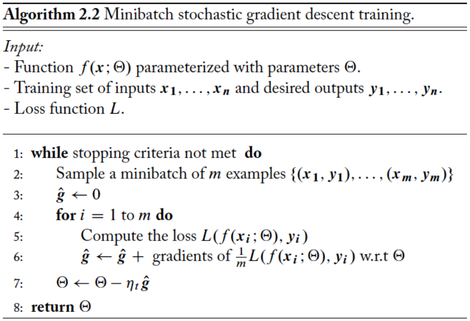
```
1: while stopping criteria not met do
2:     Sample a training example $x_i$, $y_i$
3:     Compute the loss $L(f(x_i;\Theta), y_i)$
4:     $\hat{g} \leftarrow$ gradients of $L(f(x_i;\Theta), y_i)$ w.r.t $\Theta$
5:     $\Theta \leftarrow \Theta - \eta_t \hat{g}$
6: return $\Theta$
```

- 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 $\boldsymbol{x_1},\dots,\boldsymbol{x_n}$ and desired outputs $\boldsymbol{y_1},\dots,\boldsymbol{y_n}$.
- Loss function L.

```
1: while stopping criteria not met do
2:     Sample a minibatch of $m$ examples $\{(\boldsymbol{x_1},\boldsymbol{y_1}),\dots,(\boldsymbol{x_m},\boldsymbol{y_m})\}$
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 $\Theta$
7:     $\Theta \leftarrow \Theta - \eta_t\hat{g}$
8: return $\Theta$
```

- 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 $\tilde{y}$.

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

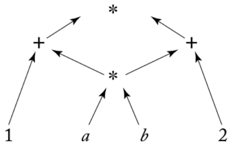
- The predicted label distribution of the categorical cross-entropy loss ($\hat{y}$) is obtained by applying the softmax function the last layer of the network $\tilde{y}$:

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

- 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

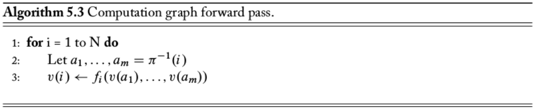
- One can compute the gradients of the various parameters of a network by hand and implement them in code.
- This procedure is cumbersome and error prone.
- For most purposes, it is preferable to use automatic tools for gradient computation [Bengio, 2012].
- A computation graph is a representation of 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

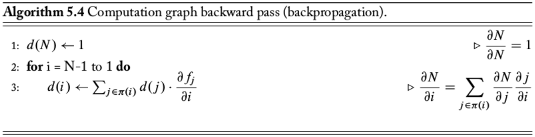
- Te computation graph abstraction allows us to:
  1. Easily construct arbitrary networks.
  2. Evaluate their predictions for given inputs (forward pass)



Algorithm 5.3 Computation graph forward pass.

```
for i = 1 to N do
    Let $a_1, \dots, a_m = \pi^{-1}(i)$
    $v(i) \leftarrow f_i(v(a_1), \dots, v(a_m))$
```

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



Algorithm 5.4 Computation graph backward pass (backpropagation).

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

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

[1] 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

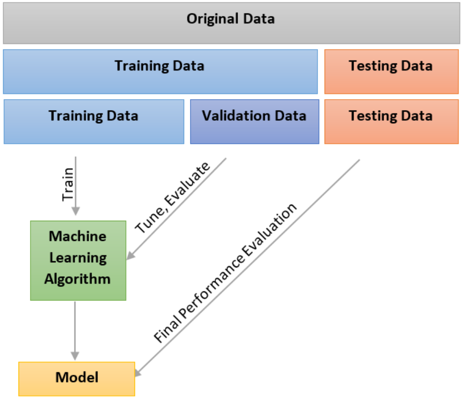
- Neural networks are prone to overfit the data.
- Hence, performance on training data can be misleading.
- Held-out set: split training set into training and testing subsets (80% and 20% splits). Train on training and compute accuracy on testing.
- Problem: in practice you often train several models, 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 [2].
- 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.

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

Train, Test, and Validation Sets



[2]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!

References I

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