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:

$$f(x) = \vec{x} \cdot W + \vec{b}$$

$$\vec{x} \in \mathcal{R}^{d_{in}} \quad W \in \mathcal{R}^{d_{in} \times d_{out}} \quad \vec{b} \in \mathcal{R}^{d_{out}}$$
(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]

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

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

 $d_{out} = 1$, \vec{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).

- 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.
- One may think that words will also be good predictors i.e., using a bag of word representation of documents.
- · Letters, or letter-bigrams are far more robust.
- We are likely to encounter a new document without any of the words we observed in the training set.
- While a document without any of the distinctive letter-bigrams is significantly less likely. [Goldberg, 2017]

- 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 \times 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.
- For example, denoting by \vec{x}_{ab} the entry of \vec{x} corresponding to the letter bigram ab:

$$x_{ab} = \frac{\#ab}{|D|} \tag{3}$$

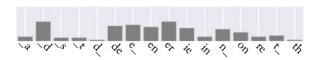
where #ab is the number of times the bigram ab appears in the document, and |D| is the total number of bigrams in the document (the document's length).



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

⁰Source:[Goldberg, 2017]

 We assume we have an alphabet of 28 letters (a–z, space, and a special symbol for all other characters including digits, punctuations, etc.)

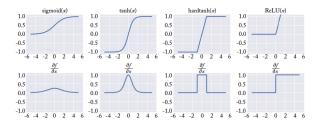


Introduction to Neural Networks

- 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.

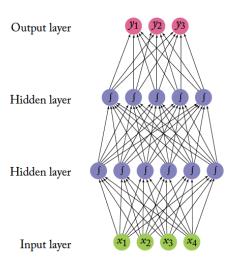
Activation Functions

- 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.



⁰Source:[Goldberg, 2016]

Feedforward Network with two Layers



⁰Source:[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_[j,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.

⁰Vectors 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:

$$NN_{MLP2}(\vec{x}) = \vec{y}$$

$$\vec{h}^{1} = g^{1}(\vec{x}W^{1} + \vec{b}^{1})$$

$$\vec{h}^{2} = g^{2}(\vec{h}^{1}W^{2} + \vec{b}^{2})$$

$$\vec{y} = \vec{h}^{2}W^{3}$$

$$\vec{y} = (g^{2}(g^{1}(\vec{x}W^{1} + \vec{b}^{1})W^{2} + \vec{b}^{2}))W^{3}.$$
(4)

Network Training

- When training a neural network one defines a loss function L(ŷ, y), stating the loss of predicting ŷ 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



⁰Source: 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 $f(x; \Theta)$ parameterized with parameters Θ .
- Training set of inputs x_1, \ldots, x_n and desired outputs y_1, \ldots, 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 $L(f(x_i; \Theta), y_i)$
- : $\hat{\mathbf{g}} \leftarrow \text{gradients of } L(f(\mathbf{x}_i; \Theta), \mathbf{y}_i) \text{ w.r.t } \Theta$
- 5: $\Theta \leftarrow \Theta \eta_t \hat{g}$
- 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).

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

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Algorithm 2.2 Minibatch stochastic gradient descent training.

Input:

- Function f(x;\Theta) parameterized with parameters \Theta.

- Training set of inputs x_1, \ldots, x_n and desired outputs y_1, \ldots, y_n.

- Loss function L.

1: while stopping criteria not met do
2: Sample a minibatch of m examples \{(x_1, y_1), \ldots, (x_m, y_m)\}
3: \hat{g} \leftarrow 0
4: for i = 1 to m do
5: Compute the loss L(f(x_i;\Theta), y_i)
6: \hat{g} \leftarrow \hat{g} + \text{gradients of } \frac{1}{m}L(f(x_i;\Theta), y_i) w.r.t \Theta
7: \Theta \leftarrow \Theta - \eta_1 \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.

⁰Source:[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 \$\tilde{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 ỹ.

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

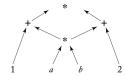
 The predicted label distribution of the categorical cross-entropy loss (ŷ) is obtained by applying the softmax function the last layer of the network ỹ:

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

• 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, ..., a_m = \pi^{-1}(i)
3: v(i) \leftarrow f_i(v(a_1), ..., v(a_m))
```

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

$$\begin{array}{ll} 1: \ d(N) \leftarrow 1 & \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \\ \triangleright \frac{\partial N}{\partial N} = 1 \\ 2: \ \ \text{for } i = N-1 \ \text{to } 1 \ \ \text{do} \\ 3: \qquad \qquad d(i) \leftarrow \sum_{j \in \pi(i)} d(j) \cdot \frac{\partial f_j}{\partial i} & \qquad \qquad \qquad \\ \triangleright \frac{\partial N}{\partial i} = \sum_{i \in \pi(i)} \frac{\partial N}{\partial j} \frac{\partial j}{\partial i} \end{array}$$

 The backpropagation algorithm (backward pass) is essentially following the chain-rule of differentiation¹.

¹A comprehensive tutorial on the backpropagation algorithm over the computational graph abstraction:

Train, Test, and Validation Sets

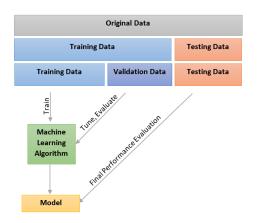
- Neural networks are prone to overfit the data.
- Hence, performance on training data can be misleading.
- Held-out set: split training set into training and testing subsets (80% and 20% splits). Train on training and compute accuracy on testing.
- Problem: in practice you often train several models, 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 sets².
- 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.

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

Train, Test, and Validation Sets



²source:

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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