Lecture 7 Deep Neural Networks

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Table of Contents

Neural Networks

Samples of cats and dogs images from Kaggle: Link

Neural Networks

- Neural Networks were first developed as models for the human brain, where we have many units (neurons) that simultaneously process signals to give a joint decision.
- The neurons fire when the total signal passed to that unit exceeds a certain threshold.
- The collective signal from all neurons tells you whether its a dog or a cat.

Neural Networks

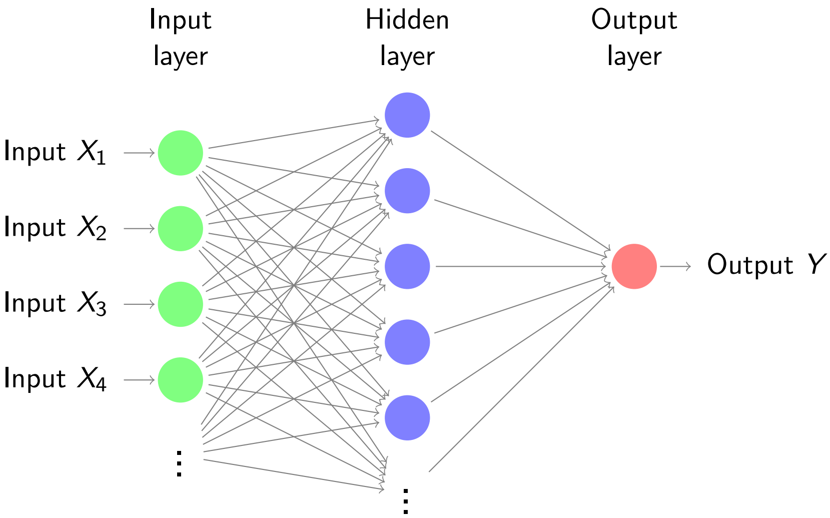


Table of Contents

Formulate the problem

- Given a training set $\{x_i, y_i\}_{i=1}^n$,
  - For regression: $y_i \in \mathbb{R}^K$ is a K dimensional continuous outcome
  - For classification: $y_i \in \{1, 2, \dots, K\}$
- The goal is still to model the relationship

$$E(Y|X) = f(X)$$

- Instead of modeling the probabilities directly using X, we build M hidden neurons as a hidden layer between X and Y:

$$\begin{aligned} Z &= (1, Z_1, Z_2, \dots, Z_M) \\ &= (1, \sigma(X^\mathsf{T}\alpha_1), \sigma(X^\mathsf{T}\alpha_2), \dots, \sigma(X^\mathsf{T}\alpha_M)) \end{aligned}$$

Formulate the problem

- $\sigma(\cdot)$ is an activation function. Some examples?
- We model Y using the hidden layer variables Z through some link function $g(\cdot)$

$$X \overset{\sigma(\cdot)}{\Longrightarrow} Z \overset{g(\cdot)}{\Longrightarrow} Y$$

- In classification problems (K class), we can use logit link g_k to model the probability of $Y = k$, for $k = 1, \dots K$:

$$g_k(Z) = \frac{\exp(Z^\mathsf{T}\boldsymbol{\beta}_k)}{\sum_{l=1}^K \exp(Z^\mathsf{T}\boldsymbol{\beta}_k)}$$

- In regression problems (could be multidimensional), we can simply use a linear function to model the kth entry of Y:

$$g_k(Z) = Z^\mathsf{T}\boldsymbol{\beta}_k$$

Formulate the problem

- The multidimensional function $\mathbf{f}(x)$ can be represented as a convoluted way of mapping $x \in \mathbb{R}^p$ to $y \in \mathbb{R}^K$

$$\mathbf{f}(x) = \mathbf{g} \circ \boldsymbol{\sigma}(x)$$

- The notations $\mathbf{g}$ and $\boldsymbol{\sigma}$ here are multidimensional.
- The parameters involved are: $\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_M$, and $\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_K$.

Examples of activation functions

- The activation function $\sigma(\cdot)$ takes a linear combination of the input variables, and output a scaler through nonlinear transformation. Examples:
  - sigmoid:

$$\sigma(v) = \frac{1}{1+e^{-v}} = \frac{e^v}{e^v+1}$$

  - hyperbolic tangent (tanh):

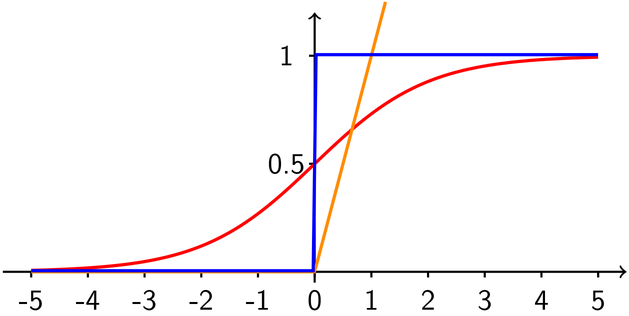
$$\sigma(v) = \frac{e^v - e^{-v}}{e^v + e^{-v}}$$

  - rectified linear unit (ReLU):

$$\sigma(v) = \max(0, v), \quad \text{soft approx.} \quad \ln(1+e^v)$$

  - And many others: exponential linear unit, arctangent, etc.

Activation Functions



Sigmoid: $(1 + e^{-v})^{-1}$
ReLU: $\max(0, v)$,
Step function: $I(v > 0)$

Activation Functions

- Originally, a step function $I(v > 0)$ was considered as the activation function (to mimic the biological interpretation). Hence for each neuron, signal is triggered only when $x^{\mathsf{T}}\alpha$ is above a certain threshold
- It was later recognized that the step function is not smooth enough for optimization, hence was replaced by a smoother threshold function, the sigmoid function
- "Feedforward" as signals can only pass to the next layer. There is no "cycle" in the model

Why Neural Networks work

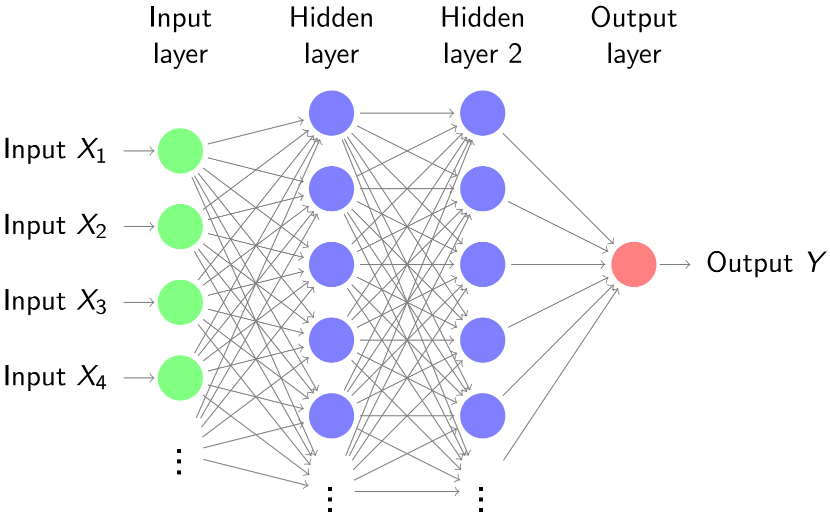
Universal Approximation Theorem (Cybenko, 1989; Hornik 1991)

Any continuous function $f(x)$ on the space $[0,1]^p$ can be approximated (for any $\varepsilon > 0$) by a finite set of neurons with a bounded monotone-increasing activation function $\sigma(\cdot)$:

$$\left| f(x) - \sum_k w_k \sigma(\beta_k^{\mathsf{T}} x + b_k) \right| < \varepsilon$$

for some w_k, β_k, and b_k. Hence, the functions defined by the neurons is dense.

Multiple Layers



Neural Networks

- Try this a really cool website: http://playground.tensorflow.org/
- Implementation in Python:
  - packages: sklearn.neural_network, (TensorFlow, PyTorch)
  - MLPClassifier implements a multi-layer perceptron (MLP) algorithm for classification.
  - MLPRegressor implements a multi-layer perceptron (MLP) for regression.
  - MLP trains using Stochastic Gradient Descent, Adam, or L-BFGS.
  - Important parameters:
    - number of neurons: hidden_layer_sizes
    - activation functions: activation
    - size of minibatches: batch_size
    - solver for back-propagation: solver
    - learning step sizes: learning_rate, learning_rate_init
    - regularization: alpha

Fitting Neural Networks

- The parameters (weights) $\boldsymbol{\alpha}$'s and $\boldsymbol{\beta}$'s need to be optimized.
- For a single hidden layer NN, we have

$$\{\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_M\}: \quad \text{M(p+1) weights}$$
$$\{\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_K\}: \quad \text{K(M+1) weights}$$

- where p is the number of non-intercept X features; M is the number of hidden neurons in a single layer; and K is the number of categories for classification.
- $K = 1$ if its a univariate regression problem.

Fitting Neural Networks

- Neural Networks training is based on error minimization using a Gradient Descent algorithm, known as error back-propagation.
- For K classification, we minimize Deviance:

$$-\sum_{i=1}^{n}\sum_{k}^{K}\mathbf{1}\{y_i = k\}\log f_k(x_i)$$

- For univariate regression, we minimize RSS (since g is linear):

$$\sum_{i=1}^{n}(y_i - f(x_i))^2 = \sum_{i=1}^{n}(y_i - \beta_0 - \beta_1\sigma(x^{\mathsf{T}}\boldsymbol{\alpha}_1) - \cdots\sigma(x^{\mathsf{T}}\boldsymbol{\alpha}_M))^2$$

Fitting Neural Networks

- The objective function can be written as

$$R(\boldsymbol{\theta}) = \sum_{i=1}^{n} R_i(\boldsymbol{\theta})$$

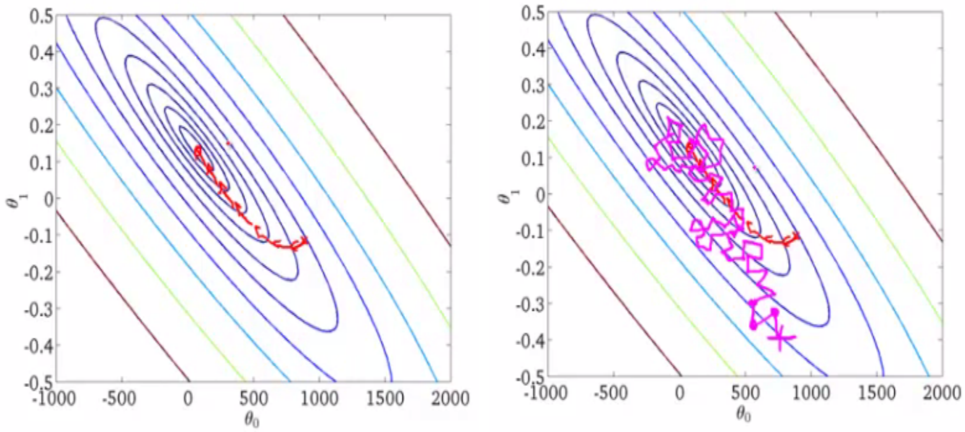
  where R_i represents the deviance or residual sum of squares for the ith data point, and $\boldsymbol{\theta}$ represents an aggregated vector of all weights
- Initiate weights $\boldsymbol{\theta}^{(0)}$
- We then calculate the derivative wrt each of the weights evaluated at the current iteration value $\boldsymbol{\theta}^{(t)}$:

$$\sum_{i=1}^{n} \frac{\partial R_i}{\beta_{km}}\bigg|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}} \qquad \sum_{i=1}^{n} \frac{\partial R_i}{\alpha_{mj}}\bigg|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}}$$

- Stochastic GD: the summation can be taken over a random subset of the n samples

GD vs. Stochastic GD

Gradient Descent vs. Stochastic Gradient Descent



Fitting Neural Networks

- The derivatives for $K = 1$ regression case is essentially

$$\frac{\partial R_i}{\beta_m} = -2(y_i - f(x_i))z_{mi}$$
$$\frac{\partial R_i}{\alpha_{ml}} = -2(y_i - f(x_i))\beta_m \sigma'(\boldsymbol{\alpha}_m^T x_i) x_{il}$$

- Some redundant calculations can be saved in the above equations. The property is called back-propagation.
- We then do the update, at the t-th iteration

$$\beta_m^{(t+1)} = \beta_m^{(t)} - \gamma \sum_{i=1}^n \frac{\partial R_i}{\beta_m^{(t)}}$$

$$\alpha_{ml}^{(t+1)} = \alpha_{ml}^{(t)} - \gamma \sum_{i=1}^n \frac{\partial R_i}{\alpha_{ml}^{(t)}}$$

where γ is a step size for gradient descent.

Fitting Neural Networks

- The derivatives can be calculated by Chain Rules
- The algorithm can be implemented by a forward-backward sweep over the network
- In the forward pass, compute the hidden variables and the output $\widehat{f}(x_i)$ based on the current weights $\boldsymbol{\theta}^{(t)}$
- In the backward pass, compute the derivatives, and update $\boldsymbol{\theta}^{(t)} \to \boldsymbol{\theta}^{(t+1)}$

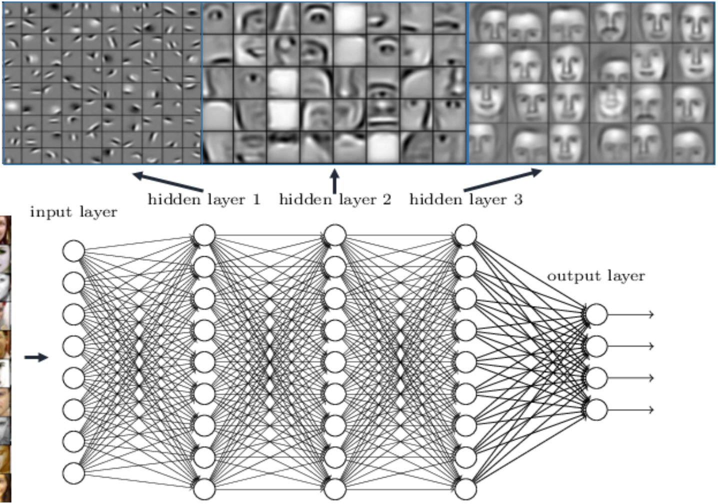
Table of Contents

Going Deeper...

- Deep Neural Networks are one type of deep learning models.
- Deep neural Networks are just ... Neural Networks with more than one hidden layer.
- But neural networks have been around for more than 70 years... why it gets popular just in recent years?
  - computational issues
  - a better way to generate/construct features
  - ...

Deep Neural Networks

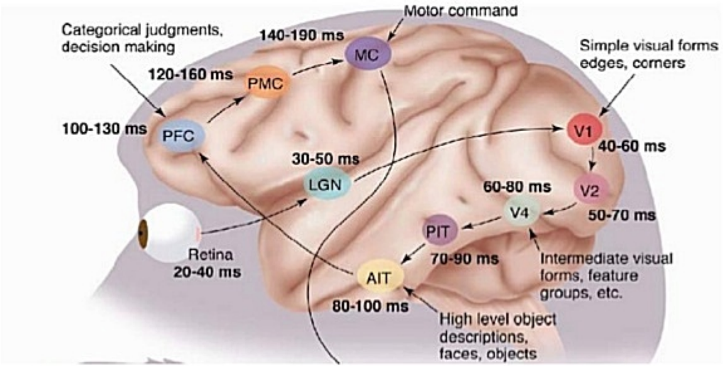
Deep neural networks learn hierarchical feature representations



Convolutional Neural Networks

- One example is the Convolutional Neural Networks, which attempts to generate better features
- Instead of using all input features to create the linear combination, a "convolutional layer" builds neurons that each takes a subset (a local region) of the input features.
- This is motivated by the fact that biologically, the neurons only take signals from neighboring neurons.

Deep Neural Networks: Feature Hierarchy



Hierarchical information processing in the brain

(Source: Simon Thorpe)

Convolutional Neural Networks

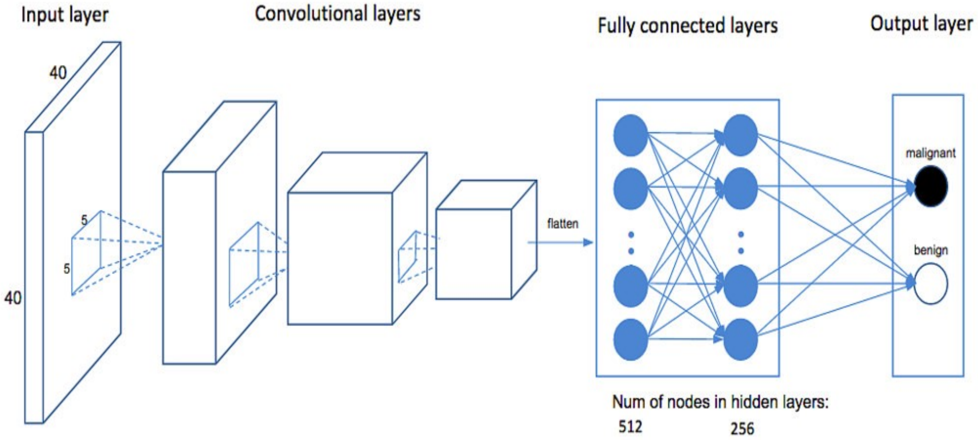
Deep Neural Networks

S.Lan

Motivation

Feedforward neural network

Deep Neural Networks



See this hand digit writing recognition example, and this interesting application by Tesla.