Slides:

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Neural Networks

Machine Learning Workshop Series

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Theory

Problem Definition

Provided a set $\mathcal{S}$ of (x_i, y_i) pairs:

$$\mathcal{S} = \{(x_1, y_1), (x_2, y_2), ..., (x_k, y_k)\}$$

Find a function f that maps $x_i \rightarrow y_i$:

$$f : \mathcal{X} \rightarrow \mathcal{Y}$$

f is a:

- **(Discriminate) Model**
- **Map Function**
- **Function Approximation**

for $\mathcal{S}$, such that:

$$f(x_i) = \hat{y}_i \approx y_i, \quad \forall i$$

Storage vs. Approximation

Map (`hashmap`, `dict`, `hash table`)

$$f[xi] \leftarrow yi$$

Suitable for:

- Finite space
- Data storage

Model (`Neural Network`, `Gaussian Process`, etc)

$$f(xi) \approx yi$$

Suitable for:

- **Infinite** space
- Function approximation

Linear Model

f is a **Linear Model**, iff:

Math

For a finite $\mathcal{S}$ where $|\mathcal{S}| = k$:

$$f(\mathbf{X}) = \hat{\mathbf{y}} = \mathbf{X} * \mathbf{w} + \mathbf{b} \tag{1}$$

where: $\mathbf{X} \in \mathbb{R}^{k \times n}$; $\hat{\mathbf{y}} \in \mathbb{R}^{k \times m}$; $\mathbf{w} \in \mathbb{R}^{n \times m}$; $\mathbf{b} \in \mathbb{R}^{m}$

Graph

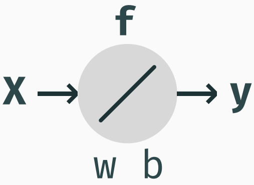


Figure 1: Linear Activation Function Neuron

f is a **Neural Network**, iff:

Math

For a finite $\mathcal{S}$ where $|\mathcal{S}| = k$:

$$f(\mathbf{X}) = \hat{\mathbf{y}} = \boldsymbol{\sigma}(\mathbf{X} * \mathbf{w_1} + \mathbf{b_1}) * \mathbf{w_2} + \mathbf{b_2} \tag{2}$$

where: $\mathbf{X} \in \mathbb{R}^{k \times n}$; $\hat{\mathbf{y}} \in \mathbb{R}^{k \times m}$; $\mathbf{w_1} \in \mathbb{R}^{n \times c}$; $\mathbf{b_1} \in \mathbb{R}^{c}$; $\mathbf{w_2} \in \mathbb{R}^{c \times m}$; $\mathbf{b_2} \in \mathbb{R}^{m}$

Graph

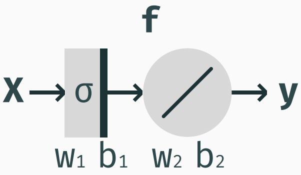


Figure 2: Single Hidden Layer Neural Network

Universal Approximation Theorem

Statement (`Existence Theorem`)

Any function can be approximated with **arbitrary precision** by some single hidden layer neural network.

Attention

This theorem does not suggest any systematic way of finding such a network, just a proof that it exists. There are other methods, such as:

- **Backpropagation Algorithm**
- general **Evolutionary Algorithms**

that are used for finding a neural network that satisfy this.

Mini Demo

Training i

- **Loss Function** $\mathcal{L}$: choose a loss function to evaluate the model.

$$\mathcal{J}(\mathbf{w}, \mathbf{b}) = \mathcal{L}(\mathbf{y} - f(\mathbf{x_i}; \mathbf{w}, \mathbf{b}))$$

Application	Loss Function
Regression	**Mean Squared Error** (MSE)
Multi-class Classification	**Cross Entropy Error**

Table 1: Choosing Loss Function $\mathcal{L}$

- **Stochastic Gradient Descent**: minimize $\mathcal{J}$ with respect to $\mathbf{w}, \mathbf{b}$.

$$\mathbf{w}^{(\mathbf{t+1})} = \mathbf{w}^{(\mathbf{t})} + \eta \frac{\partial \mathcal{J}}{\partial \mathbf{w}} \quad \text{and} \quad \mathbf{b}^{(\mathbf{t+1})} = \mathbf{b}^{(\mathbf{t})} + \eta \frac{\partial \mathcal{J}}{\partial \mathbf{b}}$$

Training ii

- **Backpropagation Algorithm**: efficient calculation of:

$$\frac{\partial \mathcal{J}}{\partial \mathbf{w_i}} \quad \text{and} \quad \frac{\partial \mathcal{J}}{\partial \mathbf{b_i}}$$

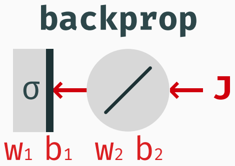


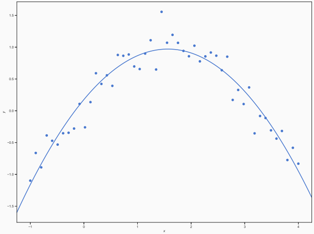
Figure 3: Backpropagation Algorithm

Backpropagation Algorithm relies on **Chain Rule**, reversing the computation of the gradients and caching them for efficient calculation of the gradients of the previous layers.

Application

Context

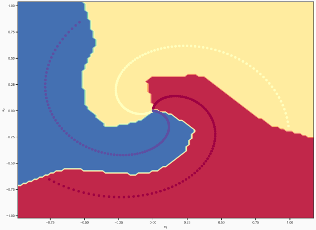
Regression



$$y \in \mathcal{R}$$

where $\mathcal{R}$ is a **continuous** set.

Classification



$$y \in \mathcal{D}$$

where $\mathcal{D}$ is a **discrete** set.

Approach i

Dataset

1. Get data $\mathcal{S}$
2. Define:
    - features matrix $\mathbf{X} \in \mathbb{R}^{k \times n}$
    - targets matrix $\mathbf{y} \in \mathbb{R}^{k \times m}$
3. (optional) Randomly split data to **train** & **test**

Neural Network Layers

1. `input_shape = n`, where `n` the number of features (columns) of $\mathbf{X}$
2. `hidden_layer_shape = ??`
3. `output_shape = m`, where `m` the number of components of $\mathbf{y}$

Approach ii

Problem Nature

- $y \in \mathcal{D}, \quad \mathcal{D}$: **discrete** $\rightarrow$ **Classification**
- $y \in \mathcal{R}, \quad \mathcal{R}$: **continuous** $\rightarrow$ **Regression**

Loss Function

- **Classification** $\rightarrow$ **Cross Entropy Error**
- **Regression** $\rightarrow$ **Mean Squared Error**

Optimisation

1. **Stochastic Gradient Descent**
2. **Backpropagation Algorithm**

Checklist

Step	Question	Answer
1	Labeled Data?	
2	Number of features of $\mathbf{X}$	
3	Number of components of $\mathbf{y}$	
4	Size of hidden layer	
5	Problem Nature	
6	Loss Function	
7	Update Rules	
8	Accuracy	

Table 2: Application using Neural Network Checklist

Questions?

Codelab

Setup

1. Create a `Github` account.
2. Sign-in `cocalc` using your `Github` credentials.
3. Create a new project in `cocalc`.
4. Clone (green button at top RHS) in `zip` format the **Neural Networks** repository.
5. `Upload` the `zip` file to newly created `cocalc` project.
6. Click on the `zip` file and extract the compressed files.
7. Navigate to the extracted folder
   `Neural-Networks-master/notebooks/Demo.ipynb`
8. Change the `kernel` by:
   `Kernel` → `Change Kernel` → `Python 3 (Anaconda)`

Challenges

Non-Linear Regression

Regression for `Boston House-Pricing` [6] dataset using:

1. a Linear Model
2. a Single Layer Feedforward Neural Network

Computer Vision

Multi-class classification of handwritten digits for `MNIST` [5] dataset using:

1. a Linear Model
2. a Single Layer Feedforward Neural Network

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