Introduction

Computational Methods for Machine Learning

Overview

- Unsupervised and semisupervised learning
    1. Major ideas
    2. The graph Laplacian
    3. Optimization
    4. Examples

Overview

- Neural Networks
  1. Linear models and their limitation
  2. Introduction to Nonlinear Models
  3. Single Layer Neural Networks
  4. Training Algorithms for Single Layer Neural Networks
  5. Introduction to Deep Neural Networks
  6. Differentiating Deep Neural Networks
  7. Stochastic Gradient Descent and Variants
- Parametric Models/Convolution Neural Networks
  1. Introduction to Parametric Models
  2. Application of CNN: Image Segmentation
  3. CNN and their relation to PDEs

Machine Learning in 3 slides

Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to perform a specific task without using explicit instructions, relying on patterns and inference instead. (wiki)

Two main classes of ML

- Given data cluster it and detect patterns in it (unsupervised learning)
- Given data and labels, find a functional relation between them (supervised learning)

Machine Learning in 3 slides

Unsupervised learning - given the data set $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n]$ cluster the data into "similar" groups (labels).

- Helps in finding hidden patterns
- Open ended

Semisupervised - label the data based on a few examples

Machine Learning in 3 slides

Supervised learning - given the data set $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n] \in \mathcal{Y}$ and their labels $\mathbf{C} = [\mathbf{c}_1, \ldots, \mathbf{c}_n] \in \mathcal{C}$, find the relation $f : \mathcal{Y} \rightarrow \mathcal{C}$

- Models range in complexity
- Older models based on Support Vector Machines and Kernel methods
- Recently Neural Networks dominate

Deep Neural Networks: History

- Neural Networks with a particular (deep) architecture
- Exist for a long time (70's and even earlier) [10, 11, 8]
- Recent revolution - computational power and big data [1, 9, 7]
- Can perform very well with lots of data
- Applications
  - Image recognition [4, 6, 7], segmentation, natural language processing [2, 3, 5]

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- A few recent news articles:
  - Apple Is Bringing the AI Revolution to Your iPhone, WIRED 2016
  - Why Deep Learning Is Suddenly Changing Your Life, FORTUNE 2016
  - Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17

NN - A Quick Overview

Neural Networks is a data interpolator/classifier when the underlying model is unknown.

A generic way to write it is

$$\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta}).$$

- The function f is the computational model.
- $\mathbf{y} \in \mathbb{R}^{n_f}$ is the input data (e.g., an image)
- $\mathbf{c} \in \mathbb{R}^{n_c}$ is the output (e.g. class the image)
- $\boldsymbol{\theta} \in \mathbb{R}^{n_p}$ are parameters of the model f

In learning we have examples $\{(\mathbf{y}_j, \mathbf{c}_j) \ : \ j = 1, \ldots, n\}$ and the goal is to estimate or "learn" the parameters $\boldsymbol{\theta}$

Learning From Data: The Core of Science

Given inputs and outputs, how to choose f?

Option 1 (Fundamental(?) understanding): For example, Newton's formula

$$x(t) = \frac{1}{2} g t^2,$$

with unknown parameter g.

Learning From Data: The Core of Science

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Option 1 (Fundamental(?) understanding): For example, Newton's formula

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with unknown parameter g.
To estimate g observe falling object

t	x
0	0
1	4.9
2	20.1
3	44.1

What is the optimal value for g?

Learning From Data: The Core of Science

Given inputs and outputs, how to choose f?

Option 2 (Phenomenological models): For example, Archie's law - what is the electrical resistivity of a rock and how it relates to its porosity, ϕ and saturation, S_w?

$$\rho(\phi, S_w) = a\phi^{n/2} S_w^p$$

a, n, p unknown parameters

Obtaining parameters from observed data and lab experiments on rocks

Phenomenological vs. Fundamental

Fundamental laws come from understanding(?) the underlying process. They are **assumed invariant** and can therefore be predictive(?).

Phenomenological models are data driven. They "work" on some given data. Hard to know what their limitations are.

But ...

- models based on understanding can do poorly - weather, economics ...
- models based on data can sometimes do better
- how do we quantify understanding?

Generalization

Suppose that we have examples $\{\mathbf{y}_j, \mathbf{c}_j\}, \quad j = 1, \ldots, n$, a model $f(\mathbf{y}, \boldsymbol{\theta})$ and some optimal parameter $\boldsymbol{\theta}^*$.
Let $\{(\mathbf{y}_j^t, \mathbf{c}_j^t) \; : \; j = 1, \ldots, s\}$ be some test set, that was not used to compute $\boldsymbol{\theta}^*$.

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For phenomenological models, there is no reason why the model should generalize, but in practice it often does.

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Why would a model generalize poorly?

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Two common reasons:

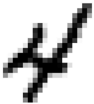
1. Our "optimal" $\boldsymbol{\theta}^*$ was optimal for the training but is less so for other data
2. The chosen computational model f is poor (e.g. linear model for a nonlinear function).

Example: Classification of Hand-written Digits

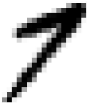
- Let $\mathbf{y}_j \in \mathbb{R}^{n_f}$ and let $\mathbf{c}_j \in \mathbb{R}^{n_c}$.
- The vector $\mathbf{c}$ is the probability of $\mathbf{y}$ belonging to a certain class. Clearly, $0 \leq \mathbf{c}_j \leq 1$ and $\sum_{j=1}^{n_c} \mathbf{c}_j = 1$.

Examples (MNIST):

$\mathbf{y}_1$



$\mathbf{y}_2$



$\mathbf{c}_1 = [0, 0, 0, 0, 1, 0, 0, 0, 0, 0]^\top$ $\mathbf{c}_2 = [0, 0.3, 0, 0, 0, 0, 0, 0.7, 0, 0]^\top$

Example: Classification of Natural Images

Image classification of natural images

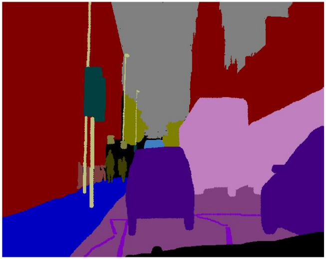
Examples (CIFAR-10):

Example: Semantic Segmentation

- let $\mathbf{y}_j \in \mathbb{R}^n$ be an RGB or grey valued image.
- let the pixels in $\mathbf{c}_j \in \{1, 2, 3, \ldots\}^k$ denote the labels.

y, input image

c, segmentation (labeled image)



Goal: Find map $\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta})$

Example 3: Semantic Segmentation

Problem: Given image $\mathbf{y}$ and label $\mathbf{c}$ find a map $f(\cdot, \boldsymbol{\theta})$ such that $\mathbf{c} \approx f(\mathbf{y}, \boldsymbol{\theta})$

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First step: Reduce the dimensionality of problem.

- extract features from the image
- classify in the feature space

Reduce the problem of learning from the image to feature detection and classification

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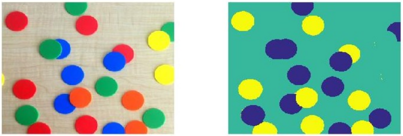
Possible features: Color, neighbors, edges ...

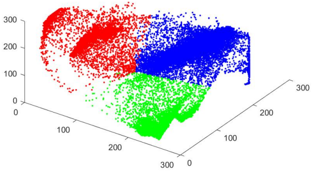
Example 3 - Semantic Segmentation

Simpler setup

- data, $\mathbf{y}$ is the RGB value of the pixel (and its neighbors?)
- $\mathbf{c}$ is a labeled pixel
- The map $\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta})$



input image and segmentation



3D representation of RGB values

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