

Problem Solving with AI Techniques

Machine Learning

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VE593, Fall 2018



JOINT INSTITUTE
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- 1 Introduction to (Supervised) Machine Learning
- 2 Supervised Learning

Introduction

What is Machine Learning?

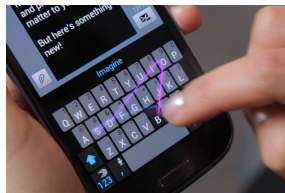
- **Machine learning:** technique that gives a computer system the ability to learn to perform a given task
- learn = improve itself as it sees more data, observations, interactions
- machine learning = "programming with data"

Why do we need Machine Learning?

- Some tasks are difficult to program
- Hand-coded programs are not adaptive

Applications

- Smart keyboard: Predict next word



- Credit scoring in finance: Predict financial health



- Visual search: Caption for an image



The man at bat readies to swing at the pitch while the umpire looks on.



A large bus sitting next to a very tall building.

Project 3: Recognizing Handwritten Digits



- Cleaned, normalized dataset of 70k images
- Hello world problem in machine learning
- One of the early success of artificial neural networks

High-level framework

The high-level framework is described as follows:

- **Goal:** learn a mapping from an input set \mathcal{X} to an output set \mathcal{Y}
 - **Given** $\mathbf{X} = (\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N)^\top, \mathbf{y} = (y^1, y^2, \dots, y^N)^\top$
 - **Assumption:** \mathbf{X}, \mathbf{y} (statistically) representative of elements in \mathcal{X}, \mathcal{Y}
-
- What are \mathbf{x} and y in the previous examples?

Classes of Learning Problems

Different classes of problems that depend on how much supervision is provided:

- Supervised Learning (\mathbf{X}, \mathbf{y})
 - Weakly-supervised Learning (inexact or inaccurate \mathbf{y})
 - Semi-supervised Learning (y^k known only for some k)
 - Reinforcement Learning
 - Unsupervised Learning (\mathbf{X} only!)
-
- Many other problems: active learning, transfer learning, multi-task learning, life-long learning....

1 Introduction to (Supervised) Machine Learning

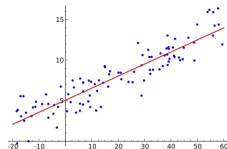
2 Supervised Learning

- Overview
- Examples of Hypothesis Classes
- Formalization

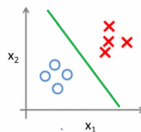
Supervised Learning

Different classes of supervised learning depending on \mathcal{Y} :

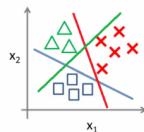
- **Regression:** For each \mathbf{x} , predict a continuous y
- **Classification:** For each \mathbf{x} , predict a discrete y
 - binary classification if $|\mathcal{Y}| = 2$
 - multi-class classification otherwise
 - Classification can be turned into regression by prediction $\mathbb{P}(Y | X)$
- **Structured prediction:** For each \mathbf{x} , predict a structured object y (e.g., sequence, tree, graph, policy...)



Binary classification:



Multi-class classification:



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Formal Framework

- **Input set** \mathcal{X}
e.g., \mathbb{R}^n , images, words
- **Output set** \mathcal{Y}
e.g., \mathbb{R} , $\{0, 1\}$, sentences, actions
- **Loss function** $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$
e.g., squared error, 0,1-loss
- **Concept class** $\mathcal{C} \subset \mathcal{Y}^{\mathcal{X}}$
e.g., linear functions from \mathcal{X} to \mathcal{Y} , Bayes nets
- **Hypothesis class** $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$
e.g., linear functions from \mathcal{X} to \mathcal{Y} , Bayes nets
- **Generative models** \mathcal{P} = set of probability distributions over $\mathcal{X} \times \mathcal{Y}$
- Why do we need a loss function? concept class? generative model?

Need for Concept Class

- Assume $\mathbf{x} \in \{0, 1\}^3$ and $y \in \{0, 1\}$
- How many functions $f : \{0, 1\}^3 \rightarrow \{0, 1\}$ are there?
- Assume we have seen the following examples. Can we generalize?

x_1	x_2	x_3	y	# consistent concepts
0	0	0	1	
0	0	1		
0	1	0		
0	1	1		
1	0	0		
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- We need an **Inductive Bias**!

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0	1	0	1	2^5
0	1	1	1	2^4
1	0	0	1	2^3
1	0	1	1	2^2
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Graphical Models

For example, using Bayes nets:

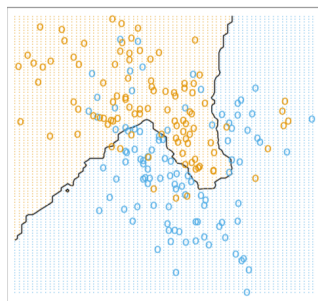
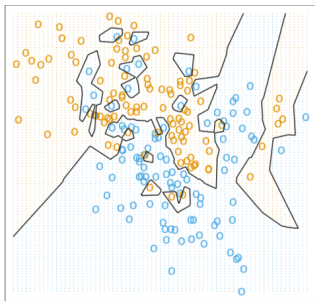
- Choose a structure (or learn from data)
- Learn parameters from data
- Use Bayes net for inference
- **Issue:** structure hard to define/learn, inference may be hard to compute for complex structure

Naive Bayes:

- **Idea:** assume that all the X^i 's are independent
- Works surprisingly well

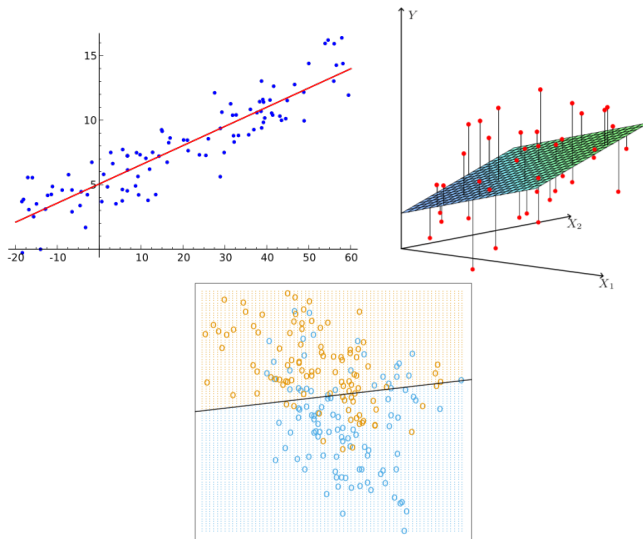
k-Nearest Neighbors

- **Principle:** for new \mathbf{x} , compute response as function of k nearest neighbors of \mathbf{x} in dataset $\mathcal{D} = \{(\mathbf{x}^i, y^i)\}$
 - Classification: majority vote
 - Regression: average
- **Issues:**
 - High computational/space requirements if dataset large
 - Doesn't scale in high dimension
 - Which distance to use?



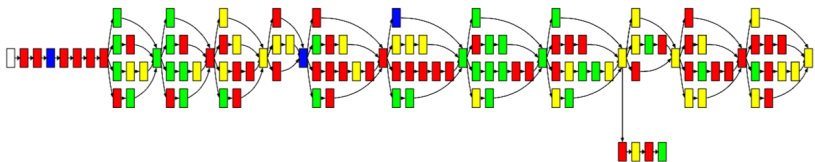
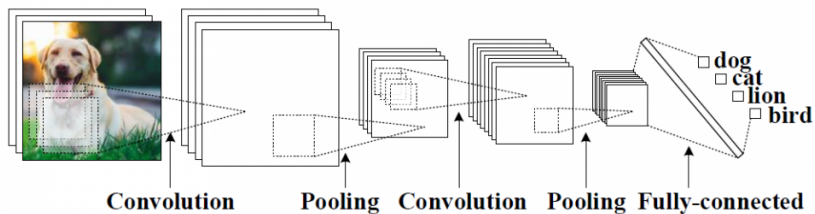
from Hastie et al.

Linear Models



from Hastie et al.

Artificial Neural Networks



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Learning Problem

- **Expected risk or error:** $R_\mu(h) = \mathbb{E}_{(X,Y) \sim \mu}[\ell(h(X), Y)]$ with $\mu \in \mathcal{P}$
- Ideally, $h^* = \arg \min_h R_\mu(h)$
- **Bayes risk:** $\min_h R_\mu(h)$
- h is **Bayes optimal** if $R_\mu(h)$ is equal to the Bayes risk
- Hard to solve because
 - μ is not known
 - optimization is over any h

Bayes Classifier

- **Expected Loss** with **0-1 Loss** $\ell(h(\mathbf{x}), y) = [h(\mathbf{x}) \neq y]$
- Expected loss is the probability of error: $R_\mu(h) = \mathbb{P}(h(X) \neq Y)$
- **Theorem.** The Bayes classifier defined as $h^*(\mathbf{x}) = \arg \max_y \mathbb{P}(y | \mathbf{x})$ reaches the Bayes error.

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- **Theorem.** The Bayes classifier defined as $h^*(\mathbf{x}) = \arg \max_y \mathbb{P}(y | \mathbf{x})$ reaches the Bayes error.
- **Proof.** For simplicity written in the discrete case:

$$h^* = \arg \min_h R_\mu(h) = \arg \min_h \sum_{\mathbf{x}} \sum_y \ell(h(\mathbf{x}), y) \mu(\mathbf{x}, y)$$

$$h^*(\mathbf{x}) = \arg \min_{y'} \sum_y \ell(y', y) \mu(\mathbf{x}, y)$$

$$h^*(\mathbf{x}) = \arg \min_{y'} \sum_{y \neq y'} \mu(\mathbf{x}, y)$$

$$h^*(\mathbf{x}) = \arg \max_{y'} \mu(\mathbf{x}, y') = \arg \max_y \mathbb{P}(\mathbf{x}, y) / \mathbb{P}(\mathbf{x})$$

Bayes Regressor

- Expected Loss with squared error loss $\ell(h(\mathbf{x}), y) = (h(\mathbf{x}) - y)^2$
- Expected loss is mean squared error: $R_\mu(h) = \mathbb{E}[(h(X) - Y)^2]$
- **Theorem.** The Bayes regressor defined as $h^*(\mathbf{x}) = \arg \max_y \mathbb{E}(y \mid \mathbf{x})$ reaches the Bayes error.

Statistical Learning Problem

- **Issue:** We don't know μ , Bayes risk cannot be reached generally
- **Idea:** given $\mathcal{D} = \{(\mathbf{x}^i, y^i) \mid i = 1, \dots, N\}$ where $(\mathbf{x}^i, y^i) \sim \mu \in \mathcal{P}$, find $H : \mathcal{X} \rightarrow \mathcal{Y} \in \mathcal{H}$ that approximately minimizes the loss $\ell(H(X), Y)$ for $(X, Y) \sim \mu$
- **Empirical Risk Minimization:** solve:

$$H^* = \arg \min_{H \in \mathcal{H}} R_{\mathcal{D}}(H) \text{ where } R_{\mathcal{D}}(H) = \sum_{i=1}^N \ell(H(\mathbf{x}^i), y^i)$$

- What are the possible issues with this approach?

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- What are the possible issues with this approach?
 - Empirical risk is only an approximation of the true risk
 - More complex hypothesis class can lead to smaller empirical risk
 - We are in fact interested in $\sum_{\mathbf{x}, y \in \mathcal{D}'} \ell(H(\mathbf{x}), y)$ where \mathcal{D}' new data set