CS 429/529
Machine Learning

Logistics

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Syllabus

- http://www.cs.unm.edu/~estrada/teaching/trilce/index.php?n=ML.Syllabus

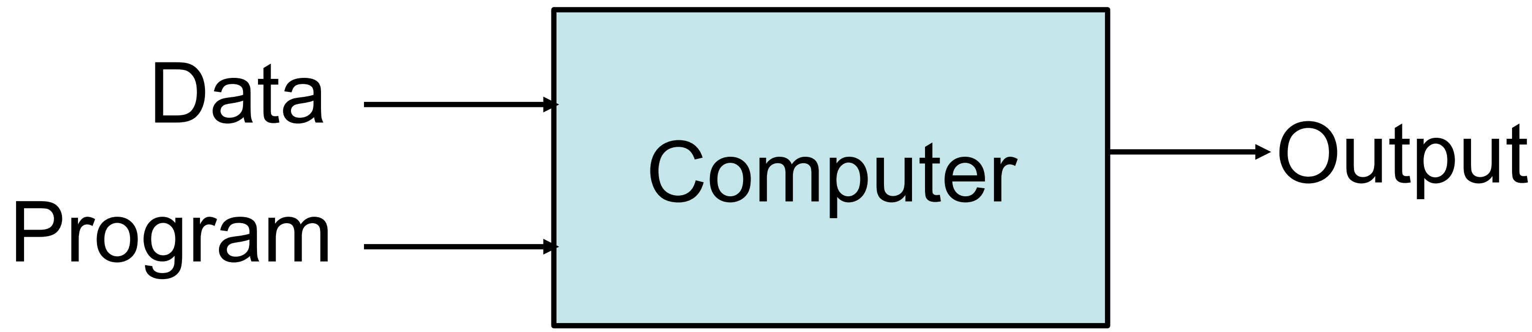
Source Materials

- T. Mitchell, ***Machine Learning,*** McGraw-Hill
- C. Bishop, ***Pattern Recognition and Machine Learning***, Springer
- Online notes (available at UNM Learn)

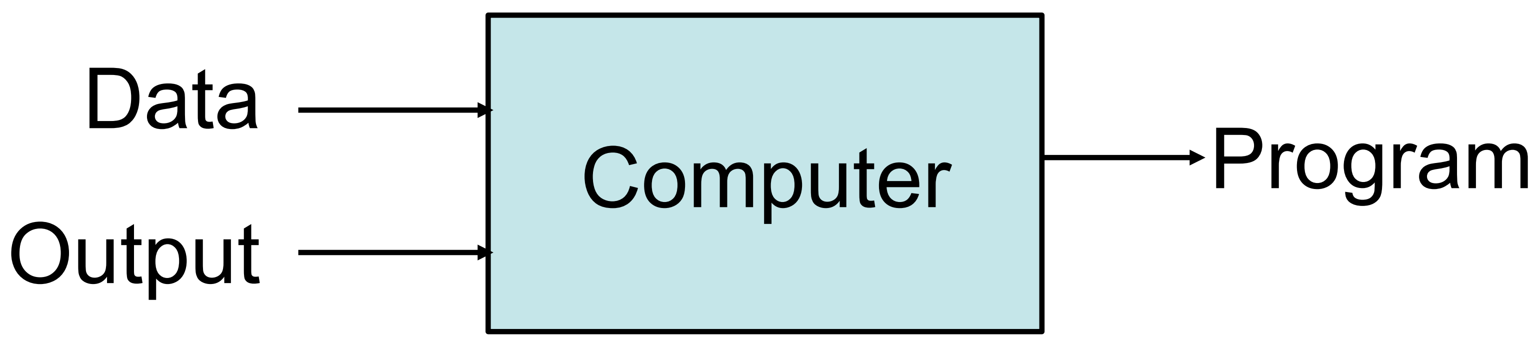
So What Is Machine Learning?

- Automating automation
- Getting computers to program themselves
- Writing software is the bottleneck
- Let the data do the work instead!

Traditional Programming



Machine Learning



Sample Applications

- Web search
- Computational biology
- Finance
- E-commerce
- Space exploration
- Robotics
- Information extraction
- Social networks
- Debugging
- [Your favorite area]

ML in a Nutshell

- Tens of thousands of machine learning algorithms
- Hundreds new every year
- Every machine learning algorithm has three components:
  - **Representation**
  - **Evaluation**
  - **Optimization**

Representation

- Decision trees
- Sets of rules / Logic programs
- Instances
- Graphical models (Bayes/Markov nets)
- Neural networks
- Support vector machines
- Model ensembles
- Etc.

Evaluation

- Accuracy
- Precision and recall
- Squared error
- Likelihood
- Posterior probability
- Cost / Utility
- Margin
- Entropy
- K-L divergence
- Etc.

Optimization

- Combinatorial optimization
  - E.g.: Greedy search
- Convex optimization
  - E.g.: Gradient descent
- Constrained optimization
  - E.g.: Linear programming

Types of Learning

- **Supervised (inductive) learning**
  - Training data includes desired outputs
- **Unsupervised learning**
  - Training data does not include desired outputs
- **Semi-supervised learning**
  - Training data includes a few desired outputs
- **Reinforcement learning**
  - Rewards from sequence of actions

Inductive Learning

- **Given** examples of a function *(X, F(X))*
- **Predict** function *F(X)* for new examples *X*
  - Discrete *F(X)*: Classification
  - Continuous *F(X)*: Regression
  - *F(X)* = Probability(*X*): Probability estimation

What We'll Cover

- **Supervised learning**
  - Decision tree induction
  - Rule induction
  - Instance-based learning
  - Bayesian learning
  - Neural networks
  - Support vector machines
  - Model ensembles
  - Learning theory
- **Unsupervised learning**
  - Clustering
  - Dimensionality reduction

Formal definition of Machine Learning

T. Mitchell: Well posed machine learning

- Improving performance via experience
- Formally, a computer program is said to learn from experience **E** with respect to some class of tasks **T** and performance measure **P**, it its performance at tasks in **T** as measured by **P**, improves with experience **E**.

Example 1: A Chess learning problem

- Task T: playing chess
- Performance measure P: percent of games won against opponents
- Training Experience E: playing practice games against itself

Example 2: Autonomous Vehicle Problem

- Task T: driving on a public highway/roads using vision sensors
- Performance Measure P: percentage of time the vehicle is involved in an accident
- Training Experience E: a sequence of images and steering commands recorded while observing a human driver

Appropriate applications for supervised learning

- Situations where:
  - There is no human expert
  - Humans can perform the task but can’t describe how they do it
  - The desired function is changing frequently
  - Each user needs a customized function

Inductive Learning

Supervised Learning

- **Given:** Training examples $\langle \mathbf{x}, f(\mathbf{x}) \rangle$ for some unknown function f.
- **Find:** A good approximation to f.

Example Applications

- **Credit risk assessment**

  $\mathbf{x}$: Properties of customer and proposed purchase.

  $f(\mathbf{x})$: Approve purchase or not.

- **Disease diagnosis**

  $\mathbf{x}$: Properties of patient (symptoms, lab tests)

  $f(\mathbf{x})$: Disease (or maybe, recommended therapy)

- **Face recognition**

  $\mathbf{x}$: Bitmap picture of person's face

  $f(\mathbf{x})$: Name of the person.

- **Automatic Steering**

  $\mathbf{x}$: Bitmap picture of road surface in front of car.

  $f(\mathbf{x})$: Degrees to turn the steering wheel.

Appropriate Applications for Supervised Learning

- **Situations where there is no human expert**

  $\mathbf{x}$: Bond graph for a new molecule.

  $f(\mathbf{x})$: Predicted binding strength to AIDS protease molecule.

- **Situations where humans can perform the task but can't describe how they do it.**

  $\mathbf{x}$: Bitmap picture of hand-written character

  $f(\mathbf{x})$: Ascii code of the character

- **Situations where the desired function is changing frequently**

  $\mathbf{x}$: Description of stock prices and trades for last 10 days.

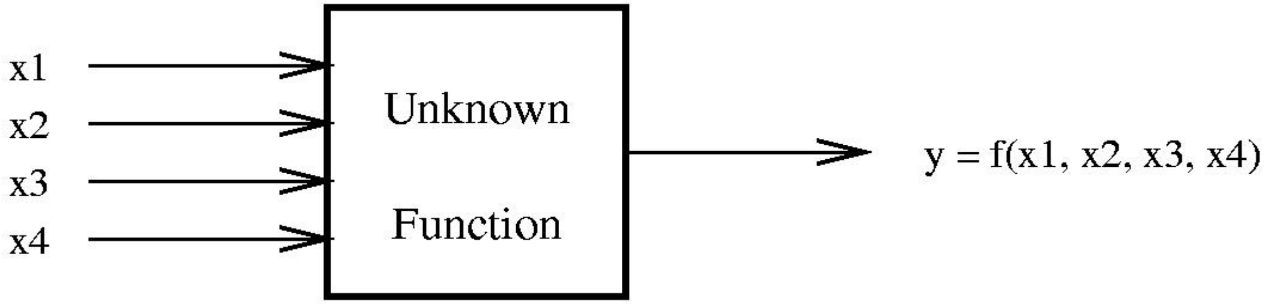
  $f(\mathbf{x})$: Recommended stock transactions

- **Situations where each user needs a customized function f**

  $\mathbf{x}$: Incoming email message.

  $f(\mathbf{x})$: Importance score for presenting to user (or deleting without presenting).

A Learning Problem



Example	x_1	x_2	x_3	x_4	y
1	0	0	1	0	0
2	0	1	0	0	0
3	0	0	1	1	1
4	1	0	0	1	1
5	0	1	1	0	0
6	1	1	0	0	0
7	0	1	0	1	0

Hypothesis Spaces

- **Complete Ignorance.** There are $2^{16} = 65536$ possible boolean functions over four input features. We can't figure out which one is correct until we've seen every possible input-output pair. After 7 examples, we still have 2^9 possibilities.

x_1	x_2	x_3	x_4	y
0	0	0	0	?
0	0	0	1	?
0	0	1	0	0
0	0	1	1	1
0	1	0	0	0
0	1	0	1	0
0	1	1	0	0
0	1	1	1	?
1	0	0	0	?
1	0	0	1	1
1	0	1	0	?
1	0	1	1	?
1	1	0	0	0
1	1	0	1	?
1	1	1	0	?
1	1	1	1	?

Hypothesis Spaces (2)

- **Simple Rules.** There are only 16 simple conjunctive rules.

Example	x_1	x_2	x_3	x_4	y
1	0	0	1	0	0
2	0	1	0	0	0
3	0	0	1	1	1
4	1	0	0	1	1
5	0	1	1	0	0
6	1	1	0	0	0
7	0	1	0	1	0

Rule	Counterexample
$\Rightarrow y$	1
$x_1 \Rightarrow y$	3
$x_2 \Rightarrow y$	2
$x_3 \Rightarrow y$	1
$x_4 \Rightarrow y$	7
$x_1 \wedge x_2 \Rightarrow y$	3
$x_1 \wedge x_3 \Rightarrow y$	3
$x_1 \wedge x_4 \Rightarrow y$	3
$x_2 \wedge x_3 \Rightarrow y$	3
$x_2 \wedge x_4 \Rightarrow y$	3
$x_3 \wedge x_4 \Rightarrow y$	4
$x_1 \wedge x_2 \wedge x_3 \Rightarrow y$	3
$x_1 \wedge x_2 \wedge x_4 \Rightarrow y$	3
$x_1 \wedge x_3 \wedge x_4 \Rightarrow y$	3
$x_2 \wedge x_3 \wedge x_4 \Rightarrow y$	3
$x_1 \wedge x_2 \wedge x_3 \wedge x_4 \Rightarrow y$	3

No simple rule explains the data. The same is true for simple clauses.

Two Strategies for Machine Learning

- **Develop Languages for Expressing Prior Knowledge:** Rule grammars and stochastic models.
- **Develop Flexible Hypothesis Spaces:** Nested collections of hypotheses. Decision trees, rules, neural networks, cases.

In either case:

- **Develop Algorithms for Finding an Hypothesis that Fits the Data**

Terminology

- **Training example.** An example of the form $\langle \mathbf{x}, f(\mathbf{x}) \rangle$.
- **Target function (target concept).** The true function f.
- **Hypothesis**. A proposed function h believed to be similar to f.
- **Concept**. A boolean function. Examples for which $f(\mathbf{x}) = 1$ are called **positive examples** or **positive instances** of the concept. Examples for which $f(\mathbf{x}) = 0$ are called **negative examples** or **negative instances.**
- **Classifier**. A discrete-valued function. The possible values $f(\mathbf{x}) \in \{1, \ldots, K\}$ are called the **classes** or **class labels**.
- **Hypothesis Space**. The space of all hypotheses that can, in principle, be output by a learning algorithm.
- **Version Space**. The space of all hypotheses in the hypothesis space that have not yet been ruled out by a training example.

A Framework for Hypothesis Spaces

- **Size**. Does the hypothesis space have a **fixed size** or **variable size**?
  Fixed-size spaces are easier to understand, but variable-size spaces are generally more useful. Variable-size spaces introduce the problem of overfitting.

- **Randomness**. Is each hypothesis **deterministic** or **stochastic**?
  This affects how we evaluate hypotheses. With a deterministic hypothesis, a training example is either *consistent* (correctly predicted) or *inconsistent* (incorrectly predicted). With a stochastic hypothesis, a training example is *more likely* or *less likely*.

- **Parameterization**. Is each hypothesis described by a set of **symbolic** (discrete) choices or is it described by a set of **continuous** parameters? If both are required, we say the hypothesis space has a **mixed** parameterization.
  Discrete parameters must be found by combinatorial search methods; continuous parameters can be found by numerical search methods.

A Framework for Learning Algorithms

- **Search Procedure**.

  Direction Computation: solve for the hypothesis directly.

  Local Search: start with an initial hypothesis, make small improvements until a local optimum.

  Constructive Search: start with an empty hypothesis, gradually add structure to it until local optimum.

- **Timing**.

  Eager: Analyze the training data and construct an explicit hypothesis.

  Lazy: Store the training data and wait until a test data point is presented, then construct an ad hoc hypothesis to classify that one data point.

- **Online vs. Batch**. (for eager algorithms)

  Online: Analyze each training example as it is presented.

  Batch: Collect training examples, analyze them, output an hypothesis.

Key Issues in Machine Learning

- **What are good hypothesis spaces?**
  Which spaces have been useful in practical applications and why?
- **What algorithms can work with these spaces?**
  Are there general design principles for machine learning algorithms?
- **How can we optimize accuracy on future data points?**
  This is sometimes called the "problem of overfitting".
- **How can we have confidence in the results?**
  How much training data is required to find accurate hypotheses? (the *statistical question*)
- **Are some learning problems computationally intractable?**
  (the *computational question*)
- **How can we formulate application problems as machine learning problems?** (the *engineering question*)