Machine Learning (CS 567) Lecture 2

Fall 2008

Time: T-Th 5:00pm - 6:20pm
Location: GFS118

Instructor: Sofus A. Macskassy (macskass@usc.edu)
Office: SAL 216
Office hours: by appointment

Teaching assistant: **Cheol Han**
Office hours: TBA

Class web page:
http://www-scf.usc.edu/~csci567/index.html

Administrative

- Email me to get on the mailing list
  - To: macskass@usc.edu
  - Subject: "csci567 student"
- Please stop me if I talk too fast
- Please stop me if you have any questions
- *Any* feedback is better than *no* feedback
  - Sooner is better
  - End of the semester is too late to make it easier on you

Administrative

- Class project info
  - Get into teams of size 2-4 as soon as you can
    - Would prefer size 2-3. See me if you want to do a project by yourself
  - I'll suggest topics in a week or two
    - Topics can be *anything* as long as it is related to ML
  - Pre-proposal due on Sep 23
    - Abstract, lay out topic and scope
  - Proposal due on Oct 9
    - 1-2 pages write up on what you will do
  - Final paper due on Dec 2
  - Presentations on Dec 2 & 4

Administrative

- Questions from last class?

Lecture 2 Outline

- Supervised learning defined
- Hypothesis spaces
- Linear Threshold Algorithms Introduction

Review: Focus for this Course

- Based on *information available*
  - Supervised – true labels provided
  - Reinforcement – Only indirect labels provided (reward/punishment)
  - Unsupervised – No feedback & no labels
- Based on the *role of the learner*
  - Passive – given a set of data, produce a model
  - Online – given one data point at a time, update model
  - Active – ask for specific data points to improve model
- Based on *type of output*
  - Concept Learning – Binary output based on +ve/-ve examples
  - Classification – Classifying into one among many classes
  - Regression – Numeric, ordered output

Supervised Learning
(and appropriate applications)

- Given: training examples <**x**, f(**x**)> for some unknown function *f*
- Find: A good approximation to f

Appropriate Applications

- There is no human expert
  - E.g., DNA analysis
    - **x**: bond graph of a new molecule
    - f(**x**): predicted binding strength to AIDS protease molecule
- Humans can perform the task but cannot explain how
  - E.g., character recognition
    - **x**: bitmap picture picture of hand-written character
    - f(**x**): ascii code of the character
- Desired function changes frequently
  - E.g., predicting stock prices based on recent trading data
    - **x**: description of stock prices and trades for last 10 days
    - f(**x**): recommended stock transactions
- Each user needs a customized function *f*
  - E.g., email filtering
    - **x**: incoming email message in some (un)structured format
    - Spam f(**x**): importance score for presenting to the user (or deleting without presenting)
    - Filter f(**x**): predicting which email folder to put the email into

Example: A data set for supervised learning

Wisconsin Breast Tumor data set from UC-Irvine Machine Learning repository.

- Thirty real-valued variables per tumor.
- Two variables that have been predicted:
  - Outcome (R=recurrence, N=non-recurrence)
  - Time (until recurrence, for R, time healthy, for N)

tumor size	texture	perimeter	…	outcome	time
18.02	27.60	117.5		N	31
17.99	10.38	122.8		N	61
20.29	14.34	135.1		R	27
…					

Terminology

tumor size	texture	perimeter	…	outcome	time
18.02	27.60	117.5		N	31
17.99	10.38	122.8		N	61
20.29	14.34	135.1		R	27
…					

- Columns are called *input variables* or *features* or *attributes*
- The outcome and time (which we are trying to predict) are called *output variables* or *targets* or *labels*
- A row in the table is called a *training example* (if used to build the model) or *instance*
- The whole table is called *(training, validation, test or evaluation) data set*

Prediction problems

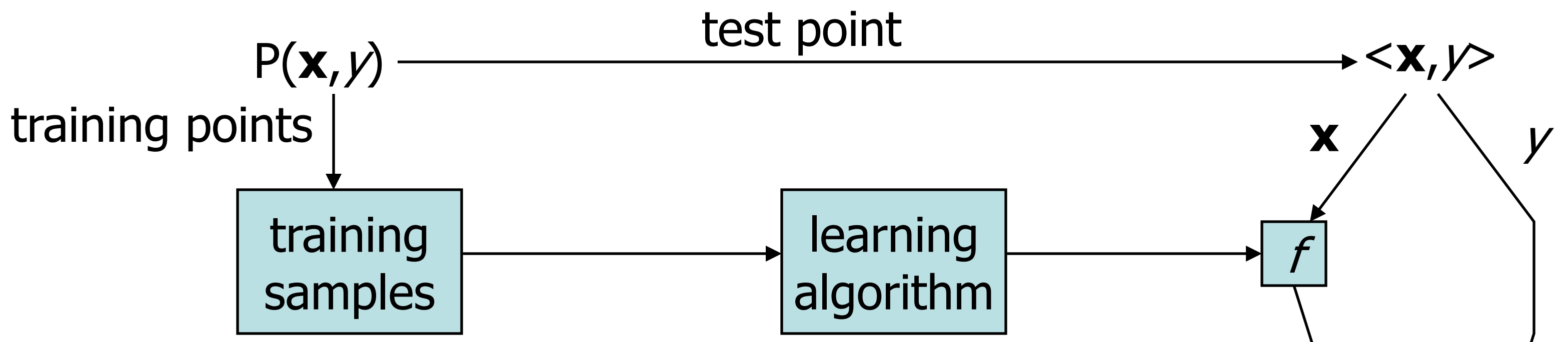
tumor size	texture	perimeter	…	outcome	time
18.02	27.60	117.5		N	31
17.99	10.38	122.8		N	61
20.29	14.34	135.1		R	27
…					

– The problem of predicting the recurrence is called *(binary) classification*
– The problem of predicting the time is called *regression*

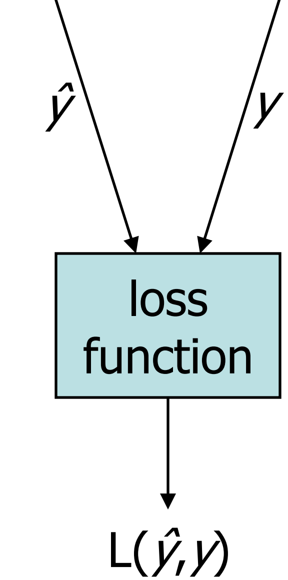
More formally

- Instances has the form: $<x_1, \ldots, x_n, y>$ where n is the number of attributes
  - We will use the notation $\mathbf{x}_i$ to denote the attributes of the i-th instances: $<x_{i,1}, \ldots, x_{i,n}>$.
- Assumptions:
  - There is underlying unknown probability distribution P($\mathbf{x}$,y), from which instances are drawn.
  - This distribution is fixed.
- Data for training as well as for future evaluation are drawn independently at random from P.
  - Instances are said to be ***i.i.d.*** (independent and identically distributed)
- Let $\mathcal{X}$ denote the space of input values
- Let $\mathcal{Y}$ denote the space of output values
  - If $\mathcal{Y} = \mathbb{R}$, this problem is called *regression*
  - If $\mathcal{Y}$ is a finite discrete set, the problem is called *classification*
  - If $\mathcal{Y}$ has 2 elements, the problem is called *binary classification* or *concept learning*

Supervised Learning Problem



- Training examples are drawn from independently at random according to unknown probability distribution $P(\mathbf{x}, y)$
- The learning algorithm analyzes the the examples and produces a classifier f or hypothesis h
- Given a new data point $\langle \mathbf{x}, y \rangle$ drawn from P (independently and at random), the classifier is given $\mathbf{x}$ and predicts $\hat{y} = f(\mathbf{x})$
- The loss $L(\hat{y}, y)$ is then measured.
- Goal of the learning algorithm: Find the f that minimizes the *expected loss.*



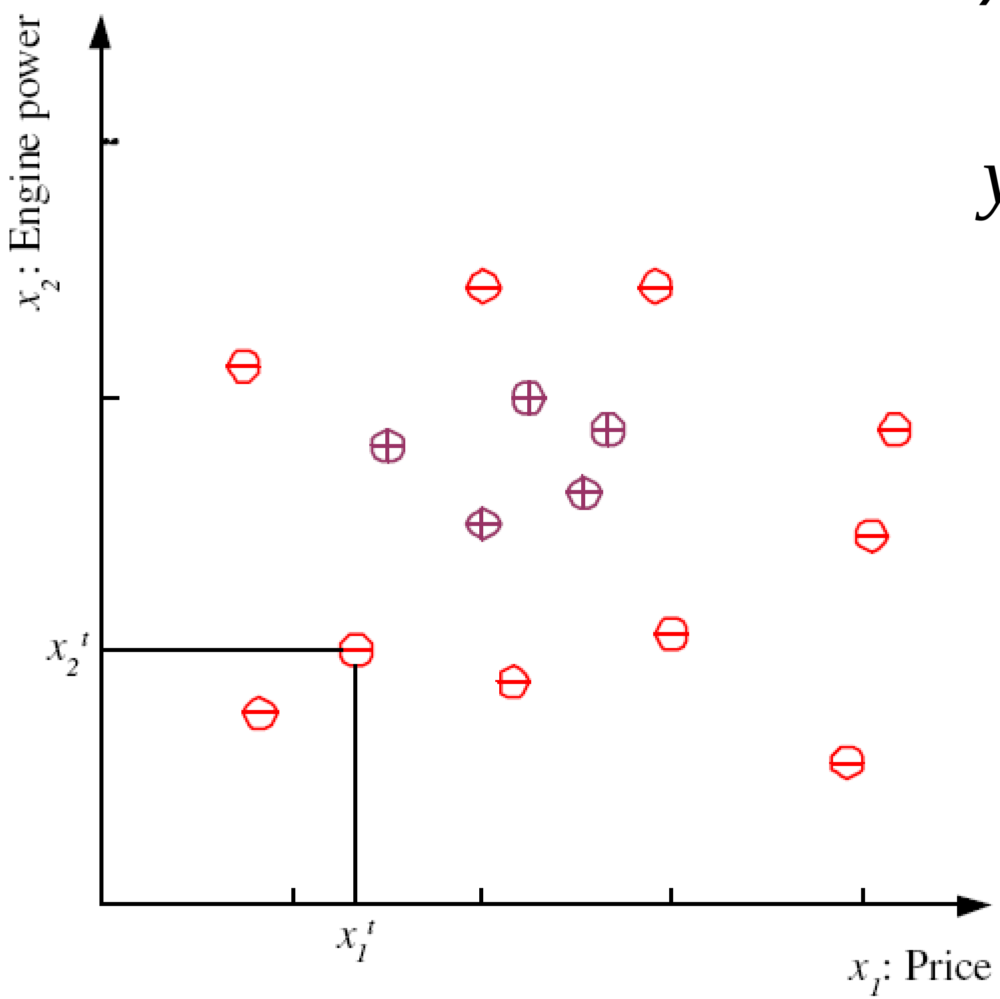
Example Problem: Family Car

- Class C of a "family car"
  - Classify: Is car x a family car?
- Output:

  Positive (+) and negative (–) examples
- Input representation:

  x_1: price, x_2 : engine power

Training set *X*



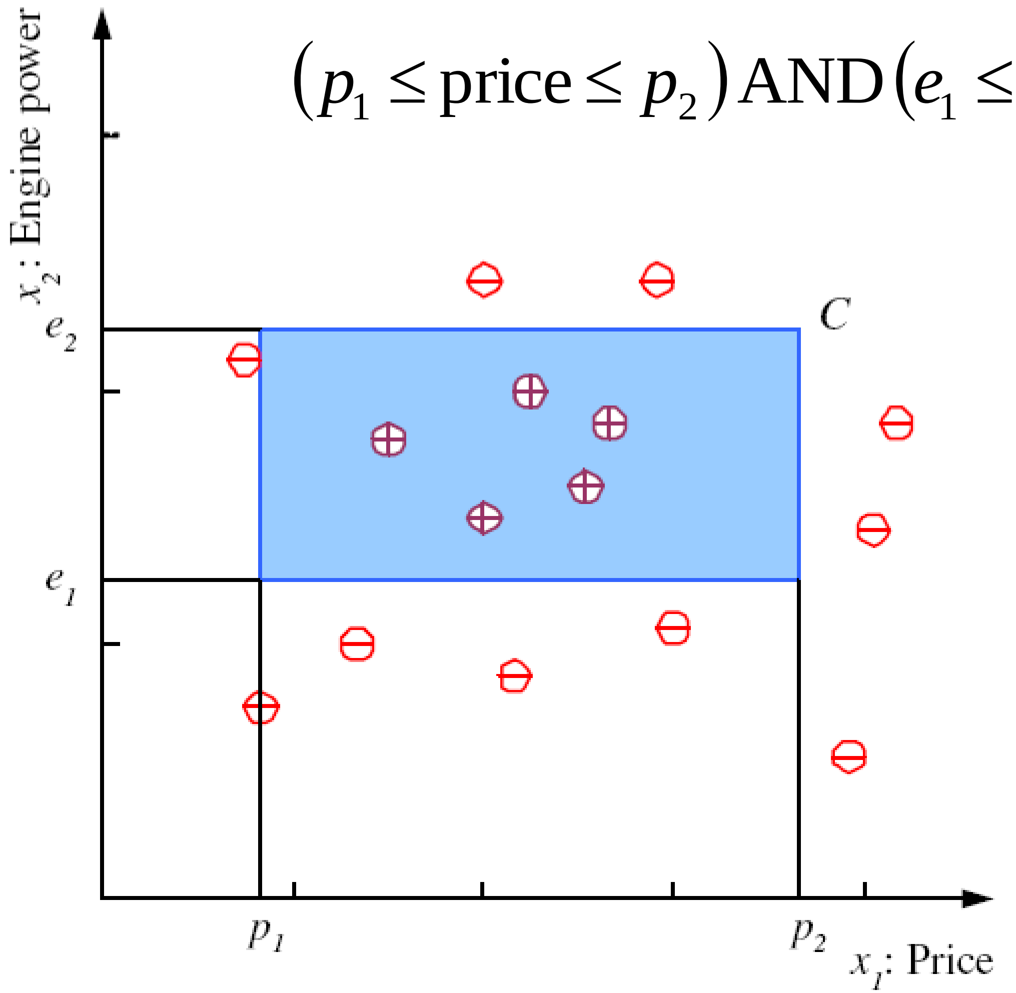
$$\mathcal{X} = \{\mathbf{x}^t, y^t\}_{t=1}^N$$

$$y = \begin{cases} 1 \text{ if } \mathbf{x} \text{ is positive} \\ 0 \text{ if } \mathbf{x} \text{ is negative} \end{cases}$$

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

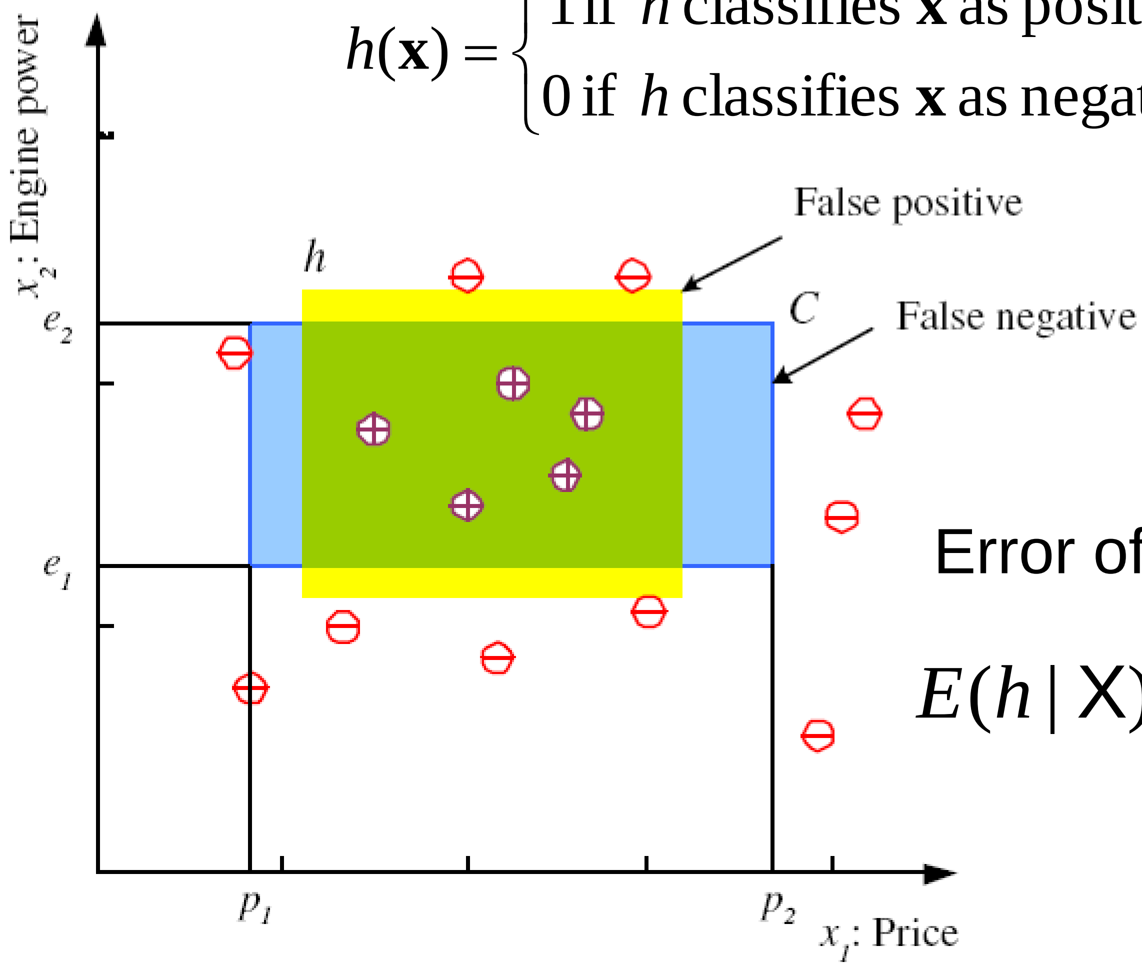
Class C

$$\left(p_1 \leq \text{price} \leq p_2\right) \text{AND} \left(e_1 \leq \text{engine power} \leq e_2\right)$$



Hypothesis class H

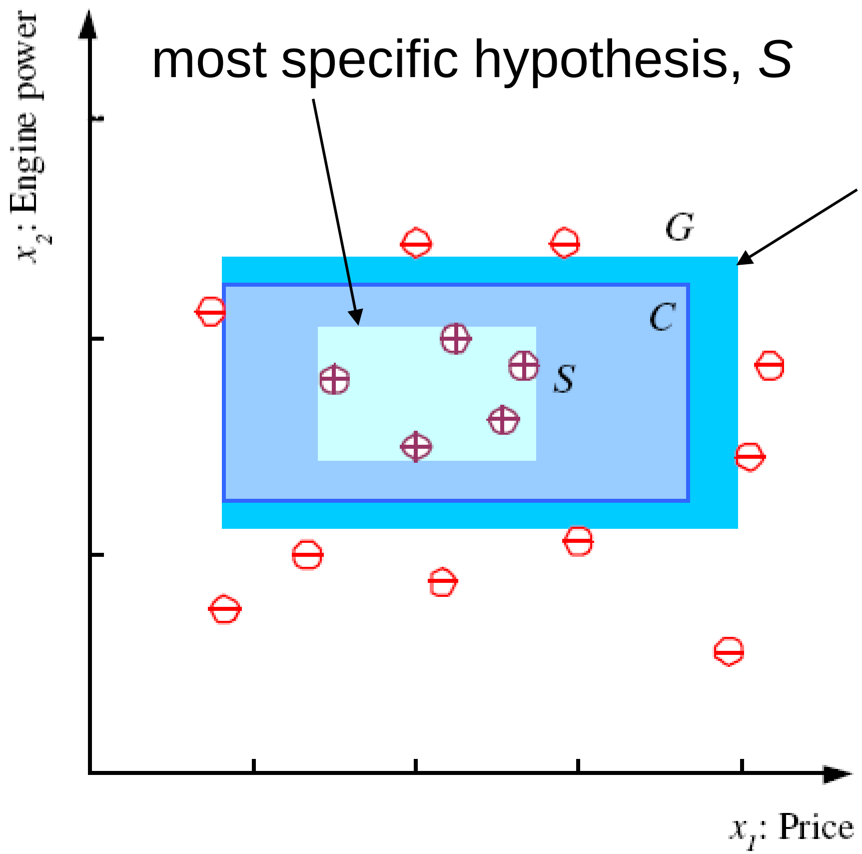
$$h(\mathbf{x}) = \begin{cases} 1 \text{ if } h \text{ classifies } \mathbf{x} \text{ as positive} \\ 0 \text{ if } h \text{ classifies } \mathbf{x} \text{ as negative} \end{cases}$$



Error of h on H

$$E(h \mid \mathrm{X}) = \sum_{t=1}^{N} 1\left(h\left(\mathbf{x}^t\right) \neq y^t\right)$$

S, G, and the Version Space



h ∈ H, between *S* and *G* is consistent

and make up the version space

(Mitchell, 1997)

Example Problem: Tumor Recurrence

- P(**x**,*y*): distribution of patients **x** and their true labels *y* ("recurrence " or "non recurrence")
- training sample: a set of patients that have been labeled by the user
- learning algorithm: that's what this class is about!
- *f* : the classifier output by the learning algorithm
- test point: A new patient **x** (with its true, but hidden, label *y*)
- loss function $L(\hat{y},y)$:

predicted label $\hat{y}$	true label y recurrence	true label y non recurrence
recurrence	0	1
non recurrence	100	0

What is $f(\mathbf{x})$?

- There are three main approaches:
  - Learn a classifier: $f: \mathcal{X} \rightarrow \mathcal{Y}$
  - Learn a conditional probability distribution: $P(y \mid \mathbf{x})$
  - Learn a joint probability distribution: $P(\mathbf{x}, y)$
- We will start by studying one example of each approach
  - Classifier: Perceptron
  - Conditional Distribution: Logistic Regression
  - Joint Distribution: Linear Discriminant Analysis (LDA)

Inferring $f(\mathbf{x})$ from $P(y|\mathbf{x})$

- Predict the $\hat{y}$ that minimizes the expected loss:

$$
\begin{aligned}
f(\mathbf{x}) &= \operatorname*{argmin}_{\hat{y}} E_{y|\mathbf{x}}[L(\hat{y}, y)] \\
&= \operatorname*{argmin}_{\hat{y}} \sum_{y} P(y|\mathbf{x}) L(\hat{y}, y)
\end{aligned}
$$

Example: Making the tumor decision

- Suppose our tumor recurrence detector predicts:

  $P(y = \text{"recurrence"} \mid \mathbf{x}) = 0.1$

  What is the optimal classification decision $\hat{y}$?
- Expected loss of $\hat{y}$ = "recurrence" is:

  $0*0.1 + 1*0.9 = 0.9$
- Expected loss of $\hat{y}$ = "non recurrence" is:

  $100*0.1 + 0*0.9 = 10$
- Therefore, the optimal prediction is "recurrence"

Loss function $L(\hat{y}, y)$:

predicted label $\hat{y}$	true label y: recurrence	true label y: non recurrence
recurrence	0	1
non recurrence	100	0
$P(y \mid \mathbf{x})$	0.1	0.9

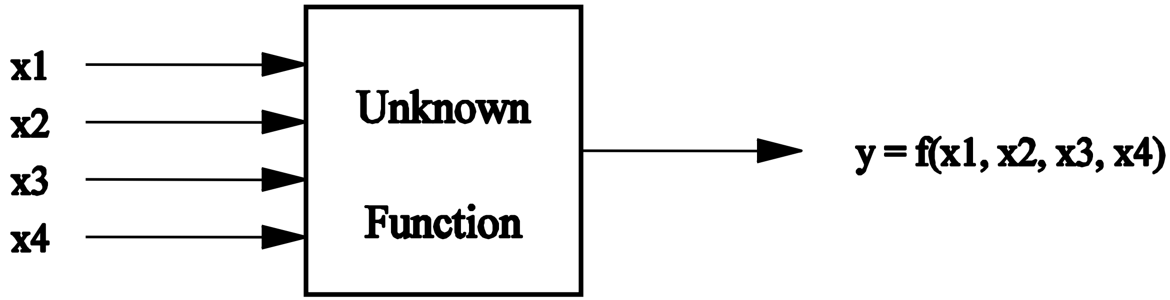
Inferring $f(\mathbf{x})$ from P($\mathbf{x}$,y)

- We can compute the conditional distribution according to the definition of conditional probability:

$$P(y = k|\mathbf{x}) = \frac{P(\mathbf{x}, y = k)}{\sum_j P(\mathbf{x}, y = j)}.$$

- In words, compute P($\mathbf{x}$, $y=k$) for each value of k. Then normalize these numbers.
- Compute $\hat{y}$ using the method from the previous slide.

Fundamental Problem of Machine Learning: It is ill-posed



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

Learning Appears Impossible

- 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	?

Solution: Work with a restricted hypothesis space

- Either by applying prior knowledge or by guessing, we choose a space of hypotheses *H* that is smaller than the space of all possible functions:
  - simple conjunctive rules
  - *m*-of-*n* rules
  - linear functions
  - multivariate Gaussian joint probability distributions
  - etc.

Illustration: Simple Conjunctive Rules

- There are only 16 simple conjunctions (no negation)
- However, no simple rule explains the data. The same is true for simple clauses

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
true $\Leftrightarrow y$	1
$x_1 \Leftrightarrow y$	3
$x_2 \Leftrightarrow y$	2
$x_3 \Leftrightarrow y$	1
$x_4 \Leftrightarrow y$	7
$x_1 \wedge x_2 \Leftrightarrow y$	3
$x_1 \wedge x_3 \Leftrightarrow y$	3
$x_1 \wedge x_4 \Leftrightarrow y$	3
$x_2 \wedge x_3 \Leftrightarrow y$	3
$x_2 \wedge x_4 \Leftrightarrow y$	3
$x_3 \wedge x_4 \Leftrightarrow y$	4
$x_1 \wedge x_2 \wedge x_3 \Leftrightarrow y$	3
$x_1 \wedge x_2 \wedge x_4 \Leftrightarrow y$	3
$x_1 \wedge x_3 \wedge x_4 \Leftrightarrow y$	3
$x_2 \wedge x_3 \wedge x_4 \Leftrightarrow y$	3
$x_1 \wedge x_2 \wedge x_3 \wedge x_4 \Leftrightarrow y$	3

A larger hypothesis space: *m*-of-*n* rules

- At least *m* of the *n* variables must be true
- There are 32 possible rules
- Only one rule is consistent!

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

	Counterexample			
variables	1-of	2-of	3-of	4-of
$\{x_1\}$	3	–	–	–
$\{x_2\}$	2	–	–	–
$\{x_3\}$	1	–	–	–
$\{x_4\}$	7	–	–	–
$\{x_1, x_2\}$	3	3	–	–
$\{x_1, x_3\}$	4	3	–	–
$\{x_1, x_4\}$	6	3	–	–
$\{x_2, x_3\}$	2	3	–	–
$\{x_2, x_4\}$	2	3	–	–
$\{x_3, x_4\}$	4	4	–	–
$\{x_1, x_2, x_3\}$	1	3	3	–
$\{x_1, x_2, x_4\}$	2	3	3	–
$\{x_1, x_3, x_4\}$	1	***	3	–
$\{x_2, x_3, x_4\}$	1	5	3	–
$\{x_1, x_2, x_3, x_4\}$	1	5	3	3

Two Views of Learning

- View 1: **Learning is the removal of our remaining uncertainty**
  - Suppose we *knew* that the unknown function was an *m*-of-*n* boolean function. Then we could use the training examples to *deduce* which function it is.
- View 2: **Learning requires <u>guessing</u> a good, small hypothesis class**
  - We can start with a very small class and enlarge it until it contains an hypothesis that fits the data

We could be wrong!

- Our prior “knowledge” might be wrong
- Our guess of the hypothesis class could be wrong
  - The smaller the class, the more likely we are wrong

Two Strategies for Machine Learning

- Develop Languages for Expressing Prior Knowledge
  - Rule grammars, stochastic models, Bayesian networks
  - (Corresponds to the Prior Knowledge view)
- Develop Flexible Hypothesis Spaces
  - Nested collections of hypotheses: decision trees, neural networks, cases, SVMs
  - (Corresponds to the Guessing view)
- In either case we must develop algorithms for finding an hypothesis that fits the data

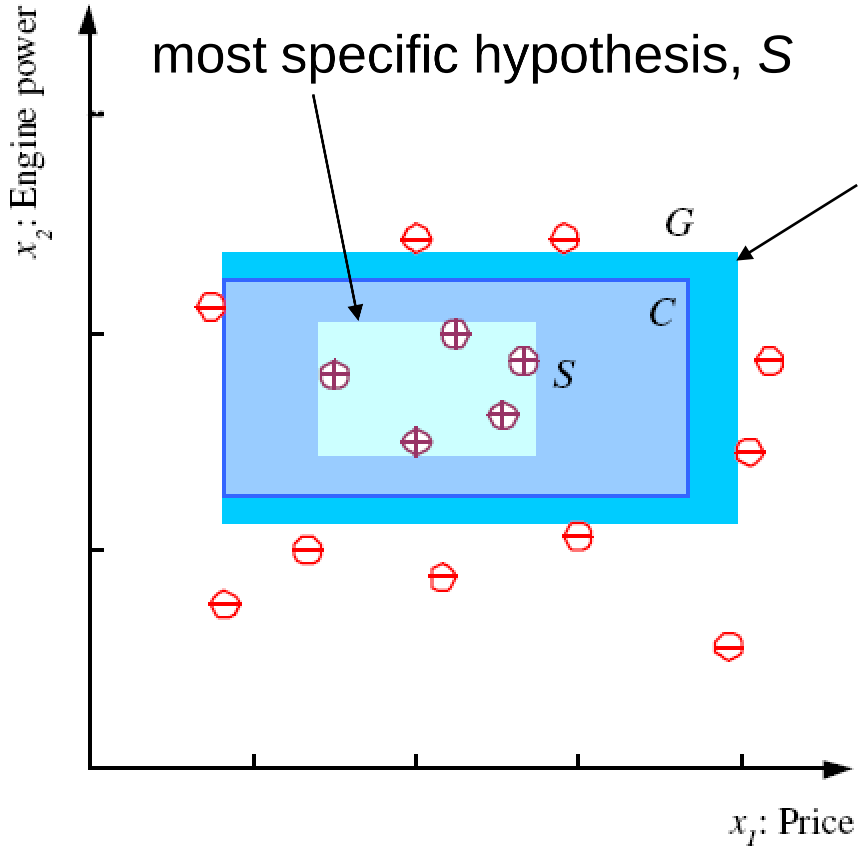
Terminology

- Training example. An example of the form $\langle \mathbf{x}, y \rangle$. $\mathbf{x}$ is usually a vector of features, y is called the class label. We will index the features by j, hence x_j is the j-th feature of $\mathbf{x}$. The number of features is n.
- Target function. The true function f, the true conditional distribution $P(y \mid \mathbf{x})$, or the true joint distribution $P(\mathbf{x}, y)$.
- Hypothesis. A proposed function or distribution h believed to be similar to f or P.
- 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.

Terminology

- 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 particular learning algorithm.
- Version Space. The space of all hypotheses in the hypothesis space that have not yet been ruled out by a training example.
- Training Sample (or Training Set or Training Data): a set of N training examples drawn according to $P(\mathbf{x}, y)$.
- Test Set: A set of training examples used to evaluate a proposed hypothesis h.
- Validation Set/Development Set: A set of training examples (typically a subset of the training set) used to guide the learning algorithm and prevent overfitting.

S, G, and the Version Space



h ∈ H, between *S* and *G* is consistent

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(Mitchell, 1997)

Key Issues in Machine Learning

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