CSCE 478/878 Lecture 2: Supervised Learning

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(Adapted from Ethem Alpaydin)

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Introduction

Supervised learning is most fundamental, "classic" form of machine learning

"Supervised" part comes from the part of *labels* for examples (instances)

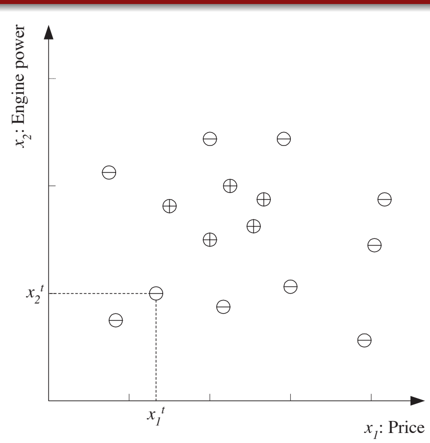
Outline

- Learning a class from labeled examples
  - Definition
  - Thinking about C
  - Hypotheses and error
  - Margin
- Noise and other problems
  - Noise
  - Model selection
  - Inductive bias
- Regression
- Multi-class problems
- General steps of machine learning

Learning a Class from Examples

- Let C be the *target concept* to be learned
  - Think of C as a function that takes as input an *example* (or *instance*) and outputs a *label*
- *Goal:* Given a *training set* $\mathcal{X} = \{(\mathbf{x}^t, r^t)\}_{t=1}^N$ where $r^t = C(\mathbf{x}^t)$, output a *hypothesis* $h \in \mathcal{H}$ that approximates C in its classifications of new instances
- Each instance $\mathbf{x}$ represented as a vector of *attributes* or *features*
  - E.g., let each $\mathbf{x} = (x_1, x_2)$ be a vector describing attributes of a car; $x_1 =$ price and $x_2 =$ engine power
  - In this example, label is binary (positive/negative, yes/no, 1/0, $+1/-1$) indicating whether instance $\mathbf{x}$ is a "family car"

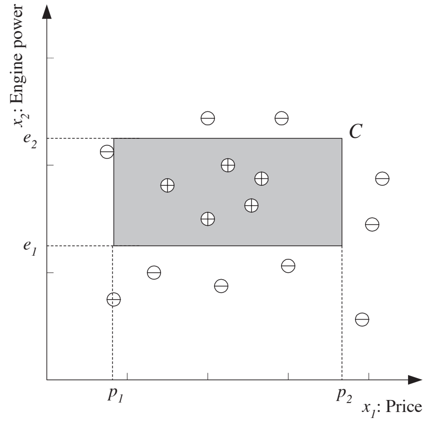
Learning a Class from Examples (cont'd)



Thinking about C

- Can think of target concept C as a *function*
  - In example, C is an axis-parallel box, equivalent to upper and lower bounds on each attribute
  - Might decide to set $\mathcal{H}$ (set of candidate hypotheses) to the same family that C comes from
  - Not required to do so
- Can also think of target concept C as a *set* of positive instances
  - In example, C the continuous set of all positive points in the plane
- Use whichever is convenient at the time

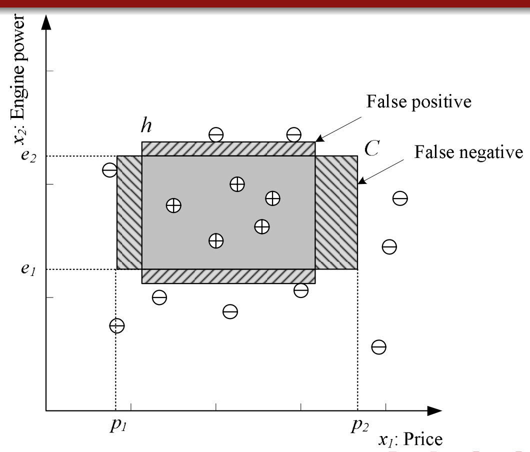
Thinking about C (cont'd)



Hypotheses and Error

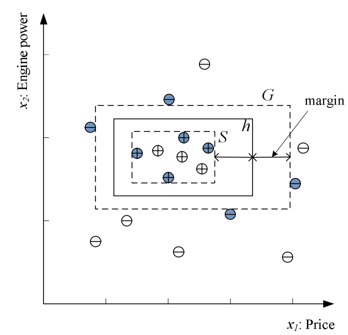
- A learning algorithm uses training set $\mathcal{X}$ and finds a hypothesis $h \in \mathcal{H}$ that approximates C
- In example, $\mathcal{H}$ can be set of all axis-parallel boxes
- If C guaranteed to come from $\mathcal{H}$, then we know that a perfect hypothesis exists
  - In this case, we choose h from the *version space* = subset of $\mathcal{H}$ consistent with $\mathcal{X}$
  - What learning algorithm can you think of to learn C?
- Can think of two types of *error* (or *loss*) of h
  - *Empirical error* is fraction of $\mathcal{X}$ that h gets wrong
  - *Generalization error* is probability that a new, randomly selected, instance is misclassified by h
    - Depends on the probability distribution over instances
  - Can further classify error as *false positive* and *false negative*

Hypotheses and Error (cont'd)



Margin

Since we will have many (infinitely?) choices of h, often will choose one with maximum *margin* (min distance to any point in $\mathcal{X}$)

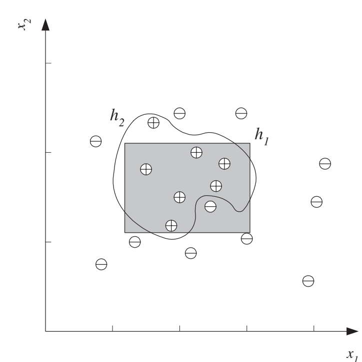


Why?

Noise and Other Problems

- In reality, it's unlikely that there exists an $h \in \mathcal{H}$ that is perfect on $\mathcal{X}$
  - Could be *noise* in the data (attribute errors, labeling errors)
  - Could be attributes that are *hidden* or *latent*, which impact the label but are unobserved
- Could find a better (or even perfect) fit to $\mathcal{X}$ if we choose a more powerful (expressive) hypothesis class $\mathcal{H}$
- Is this a good idea?

Noise and Other Problems (cont'd)



For what reasons might we prefer h_1 over h_2?

Model Selection

- Might prefer simpler hypothesis because it is:
  - Easier/more efficient to evaluate
  - Easier to train (fewer parameters)
  - Easier to describe/justify prediction
  - Better fits *Occam's Razor:* Tend to prefer simpler explanation among similar ones
- *Model selection* is the act of choosing a hypothesis class $\mathcal{H}$
  - Need to balance $\mathcal{H}$'s complexity with that of the model that labels the data:
    - If $\mathcal{H}$ not sophisticated enough, might *underfit* and not generalize well (e.g., fit line to data from cubic model)
    - If $\mathcal{H}$ too sophisticated, might *overfit* and not generalize well (e.g., fit the noise)
  - Can validate choice of h (and $\mathcal{H}$) if some data held back from $\mathcal{X}$ to serve as *validation set*
    - Still part of training, but not directly used to select h
  - Independent *test set* often used to do final evaluation of chosen h

Inductive Bias

- Must assume something about the learning task
- Otherwise, learning becomes rote memorization
- Imagine allowing $\mathcal{H}$ to be set of arbitrary functions over set of all possible instances
  - Every hypothesis in version space $\mathcal{V} \subseteq \mathcal{H}$ is consistent with all instances in $\mathcal{X}$
  - For every other instance, *exactly half* the hypotheses in $\mathcal{V}$ will predict positive, the rest negative (see next slide)
  - $\Rightarrow$ No way to generalize on new, unseen instances without way to favor one hypothesis over another
- *Inductive bias* is a set of assumptions that we make to enable generalization over rote memorization
  - Manifests in choice of $\mathcal{H}$
  - Instead (or in addition), can have bias in *preference* of some hypotheses over others (e.g., based on specificity or simplicity)

Inductive Bias (cont'd)

- E.g., if $\mathcal{X} = \{(\langle 0,0,0\rangle, +), (\langle 1,1,0\rangle, +), (\langle 0,1,0\rangle, -), (\langle 1,0,1\rangle, -)\}$ then version space $\mathcal{V}$ is the set of truth tables satisfying

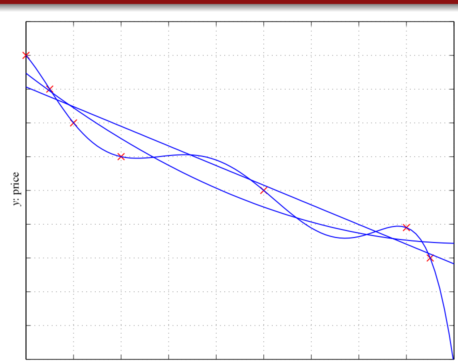
000	+	010	−	100		110	+
001		011		101	−	111	

- Since there are 4 holes, $|\mathcal{V}| = 2^4 = 16$ = number of ways to fill holes, and for any yet unclassified example $\mathbf{x}$, *exactly half* of hyps in $\mathcal{V}$ classify $\mathbf{x}$ as $+$ and half as $-$

Regression

- When labels $f(\mathbf{x})$ are real-valued rather than discrete, we call it *regression*
- Error of hypothesis g measured by *squared error* instead of number of misclassifications: $(f(\mathbf{x}) - g(\mathbf{x}))^2$
  - Empirical error is now average squared error and generalization performance is expected squared error
- Model selection now consists of choosing the complexity of hypothesis g, e.g., degree of polynomial:
  - Linear: $g(x) = w_1 x + w_0$
  - Quadratic: $g(x) = w_2 x^2 + w_1 x + w_0$
  - And so on, where higher-order polynomials can better fit data based on more complex models, but are also more inclined to overfit
- Learning consists of inferring parameters w_i

Regression (cont'd)



Polynomials of degree 1, 2, and 6

Multi-Class Problems

- Some classification problems have discrete-valued labels, but not binary
- E.g., instead of "family car" versus "not family car", have labels {"family car", "luxury sedan", "sports car"}
- How we handle this depends on the type of hypothesis/learning algorithm we use
  - Some hypothesis classes (e.g., decision trees, k nearest neighbor) naturally have the ability to classify with non-binary labels
  - Some are binary only (e.g., artificial neural networks, support vector machines, axis-parallel boxes)
    - In this case, can cast the multi-class problem as a collection of binary problems
    - In a K-class problem, can give each instance a *vector* of K binary labels

Multi-Class Problems (cont'd)

- E.g., if original training set is

$$\mathcal{Y} = \{(\mathbf{x}^t, s^t)\}_{t=1}^N$$

for each $s^t \in \{C_1, \ldots, C_K\}$, then map it to

$$\mathcal{X} = \{(\mathbf{x}^t, \mathbf{r}^t)\}_{t=1}^N$$

where each $\mathbf{r}^t$ is a K-dimensional binary vector:

$$r_i^t = \begin{cases} 1 & \text{if } \mathbf{x}^t \in C_i \\ 0 & \text{if } \mathbf{x}^t \in C_j, j \neq i \end{cases}$$

- Can then train K separate binary classifiers in *one-versus-rest* scheme
- (Other encodings of $\mathbf{r}$ also possible)

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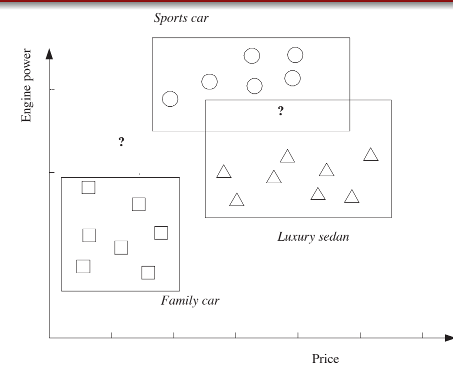
Multi-Class Problems (cont'd)



Three axis-parallel boxes as three binary classifiers, one per class

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General Steps of Machine Learning

- Acquire training set $\mathcal{X} = \{(\mathbf{x}^t, r^t)\}_{t=1}^N$
  - Assume *independent and identically distributed* (iid)
  - Assume probability distribution on $\mathcal{X}$ is same as what we will see in practice
  - Labels r^t could be binary, multi-valued, real
- Choose hypothesis class $\mathcal{H}$
- Choose loss function L
  - 0-1 loss versus hinge loss versus squared loss ...
- Choose optimization procedure to find h
  - E.g., analytic solution for linear regression, backpropagation for artificial neural network, sequential minimal optimization for SVM
- Evaluate quality of h via estimation of generalization performance using *independent test set*