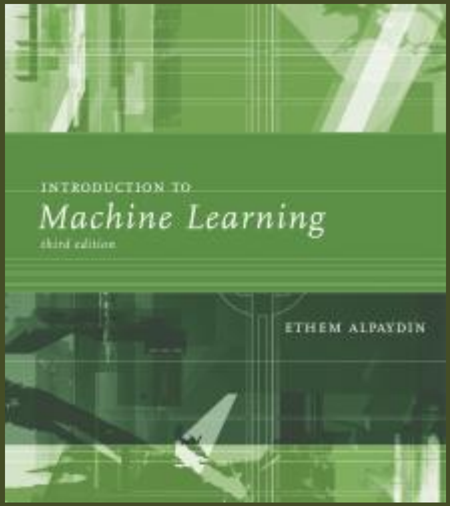

Lecture Slides for

INTRODUCTION TO MACHINE LEARNING

3RD EDITION

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CHAPTER 2:

SUPERVISED LEARNING

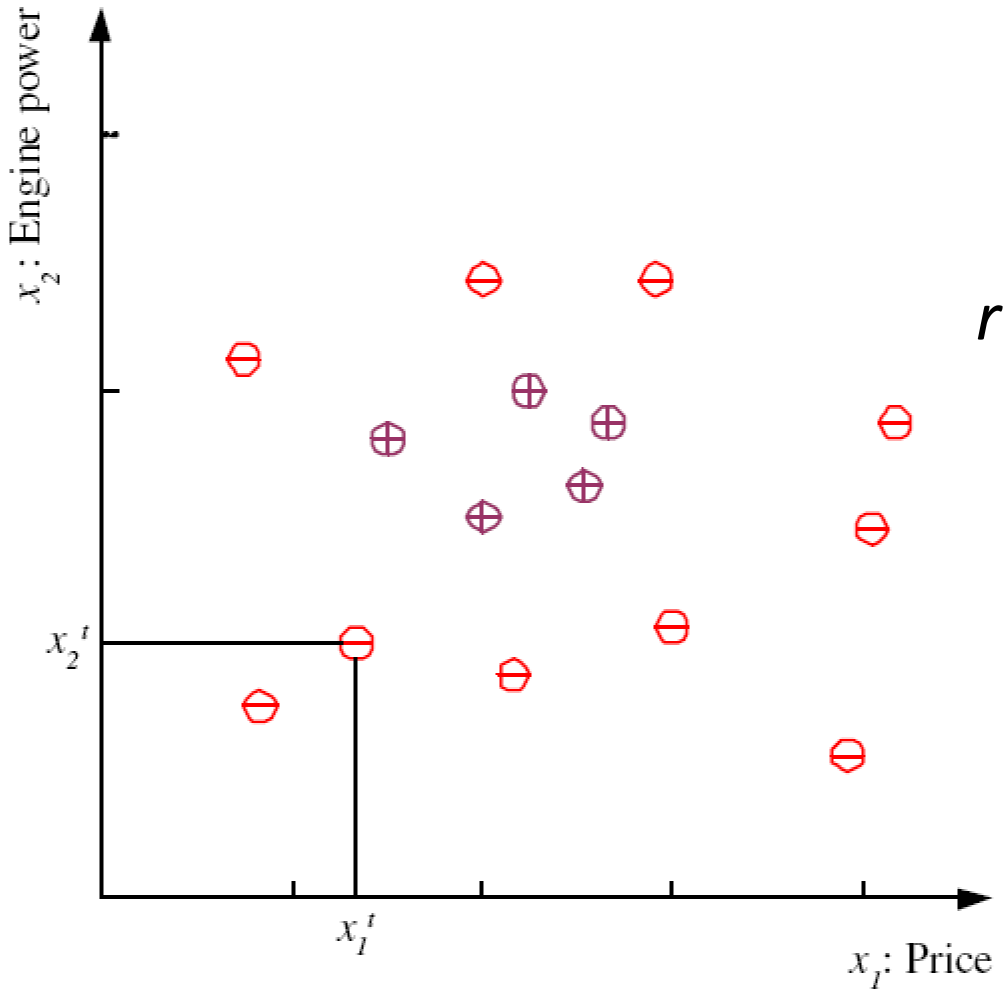
Learning a Class from Examples

- Class C of a "family car"
  - Prediction: Is car x a family car?
  - Knowledge extraction: What do people expect from a family car?
- Output:

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

  x_1: price, x_2 : engine power

Training set $\mathcal{X}$



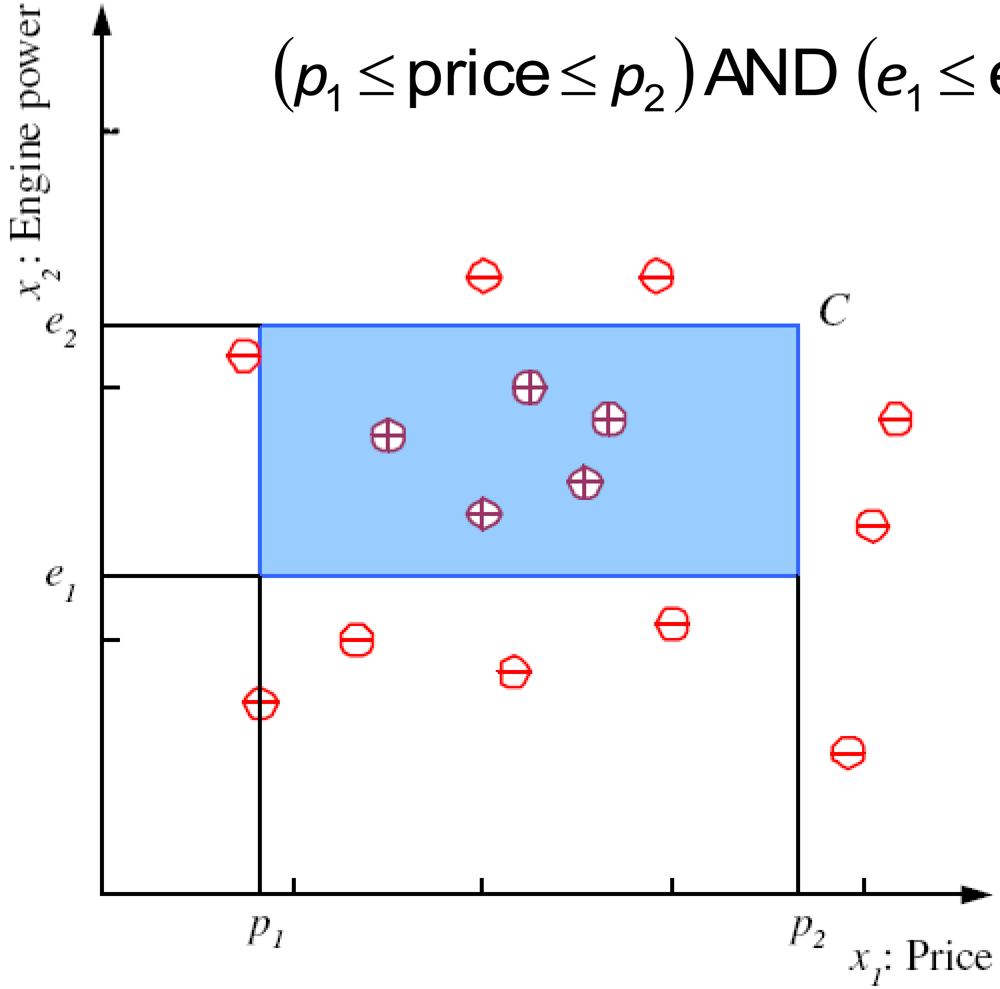
$$\mathcal{X} = \{\mathbf{x}^t, r^t\}_{t=1}^N$$

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

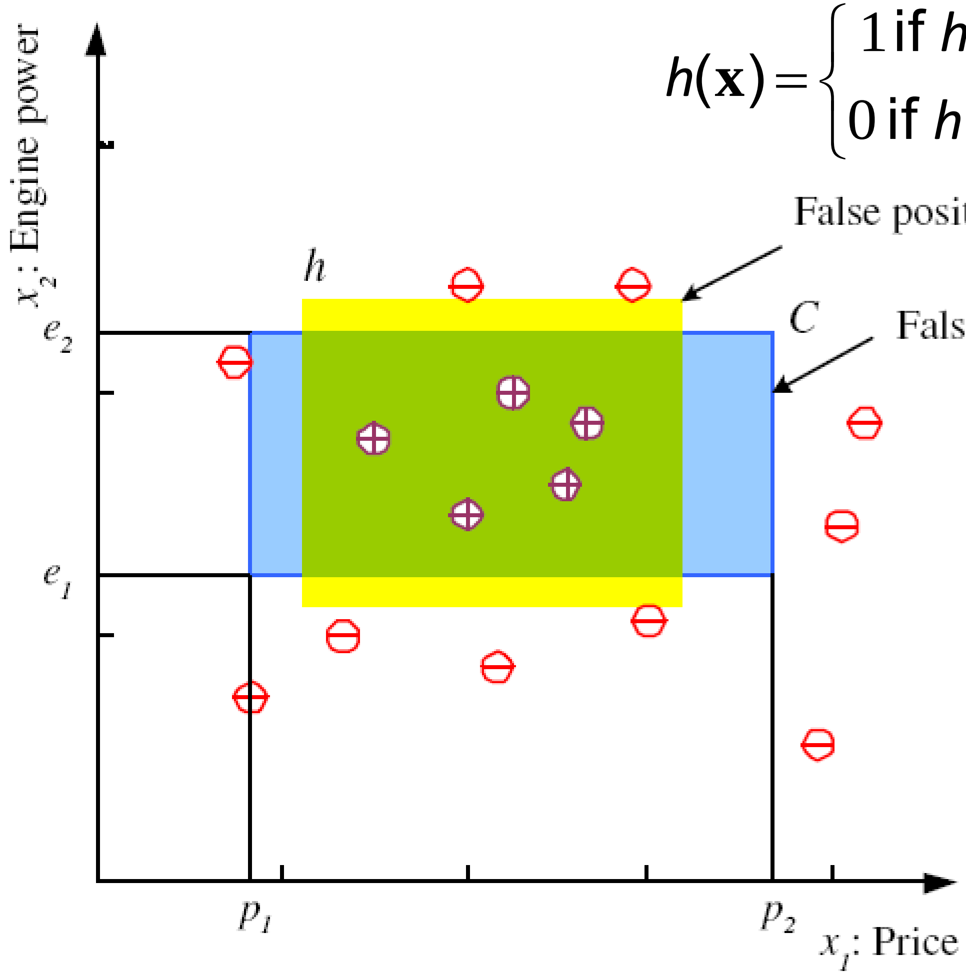
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Class C

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



Hypothesis class $\mathcal{H}$

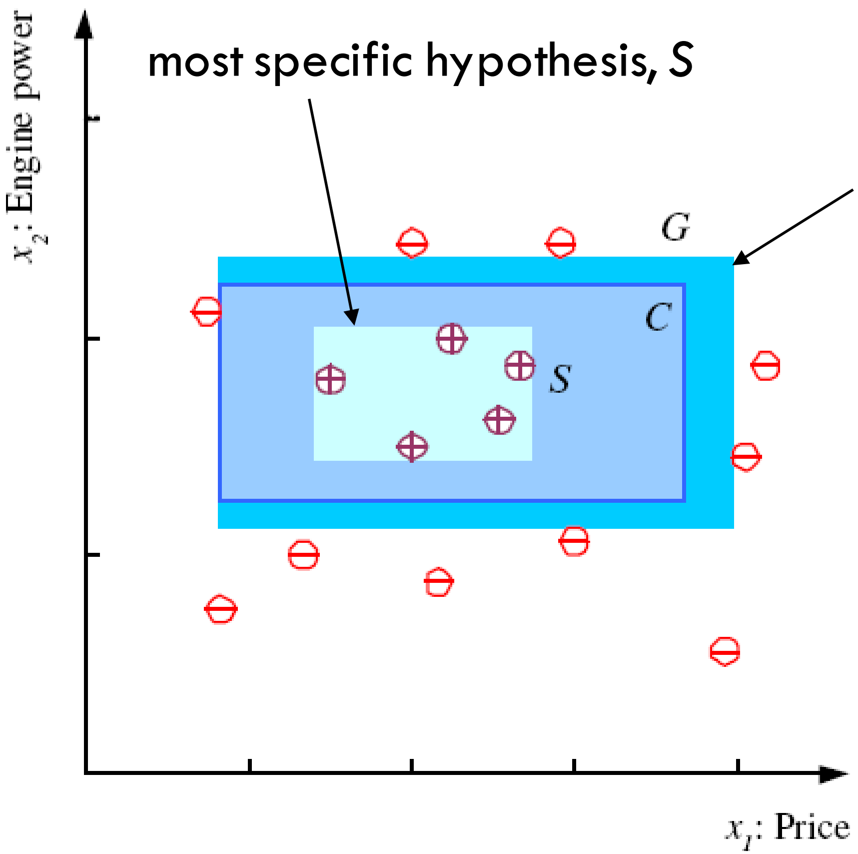


$$h(\mathbf{x}) = \begin{cases} 1 \text{ if } h \text{ says } \mathbf{x} \text{ is positive} \\ 0 \text{ if } h \text{ says } \mathbf{x} \text{ is negative} \end{cases}$$

Error of h on $\mathcal{H}$

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

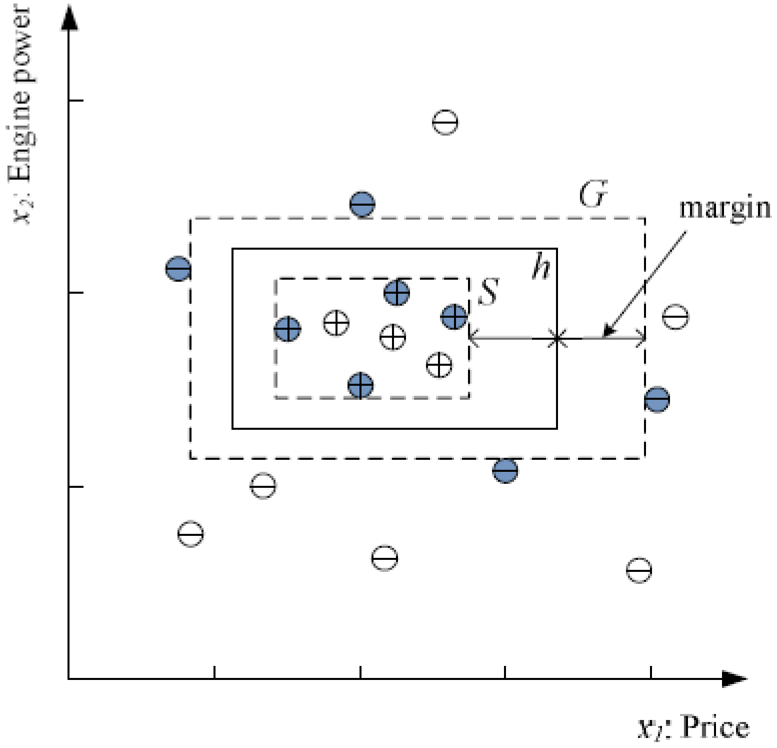
S, G, and the Version Space



$h \in$ H, between *S* and G is consistent and make up the version space
(Mitchell, 1997)

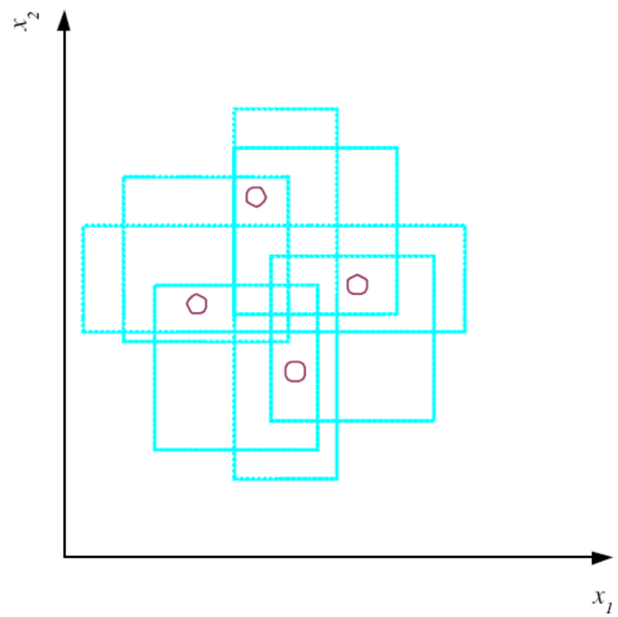
Margin

- Choose *h* with largest margin



VC Dimension

- N points can be labeled in 2^N ways as $+/-$
- $\mathcal{H}$ shatters N if there exists $h \in \mathcal{H}$ consistent for any of these: $\text{VC}(\mathcal{H}) = N$



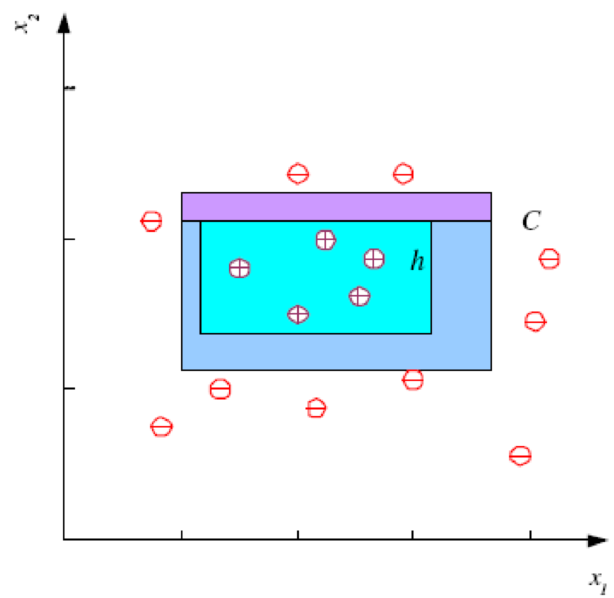
An axis-aligned rectangle shatters 4 points only !

Probably Approximately Correct (PAC) Learning

- How many training examples N should we have, such that with probability at least $1 - \delta$, h has error at most ε ?

  (Blumer et al., 1989)

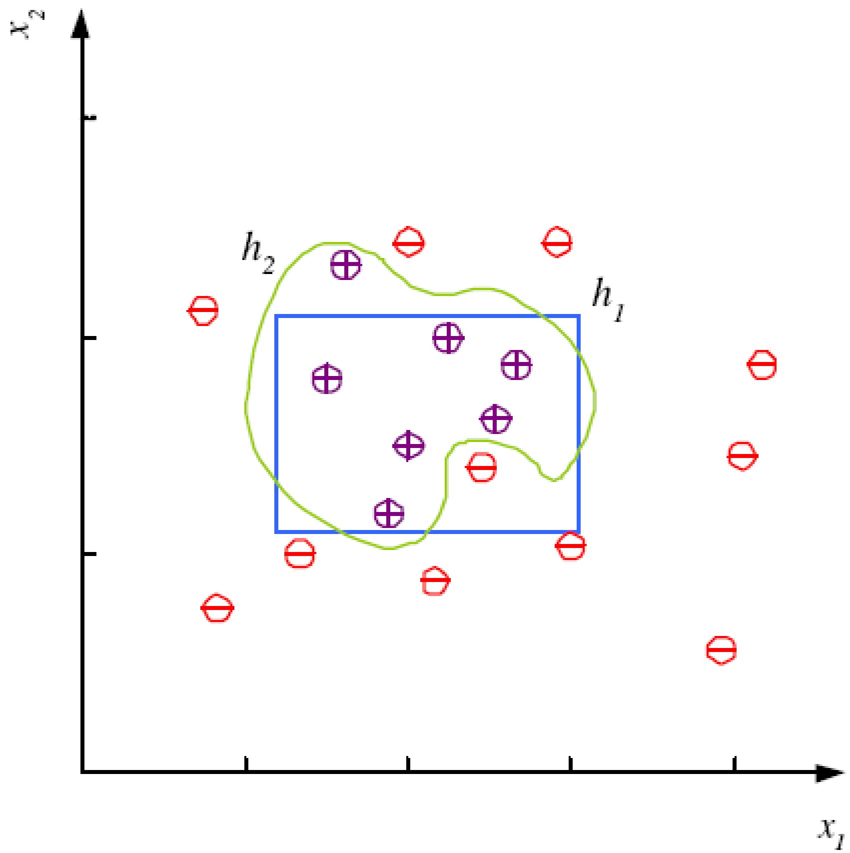
- Each strip is at most $\varepsilon/4$
- Pr that we miss a strip $1 - \varepsilon/4$
- Pr that N instances miss a strip $(1 - \varepsilon/4)^N$
- Pr that N instances miss 4 strips $4(1 - \varepsilon/4)^N$
- $4(1 - \varepsilon/4)^N \leq \delta$ and $(1 - x) \leq \exp(-x)$
- $4\exp(-\varepsilon N/4) \leq \delta$ and $N \geq (4/\varepsilon)\log(4/\delta)$



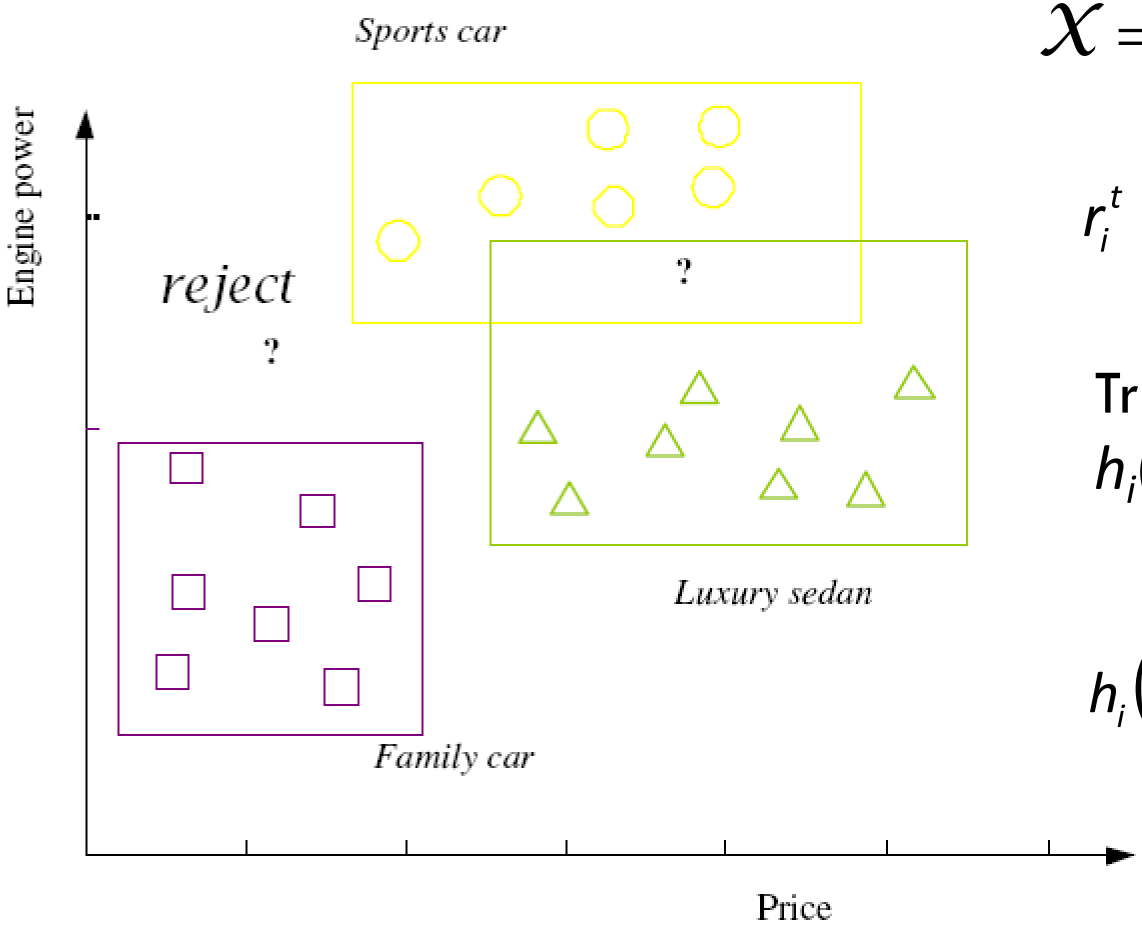
Noise and Model Complexity

Use the simpler one because

- Simpler to use (lower computational complexity)
- Easier to train (lower space complexity)
- Easier to explain (more interpretable)
- Generalizes better (lower variance - Occam's razor)



Multiple Classes, C_i i=1,...,K



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

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

Train hypotheses

$h_i(\boldsymbol{x})$, i =1,...,K:

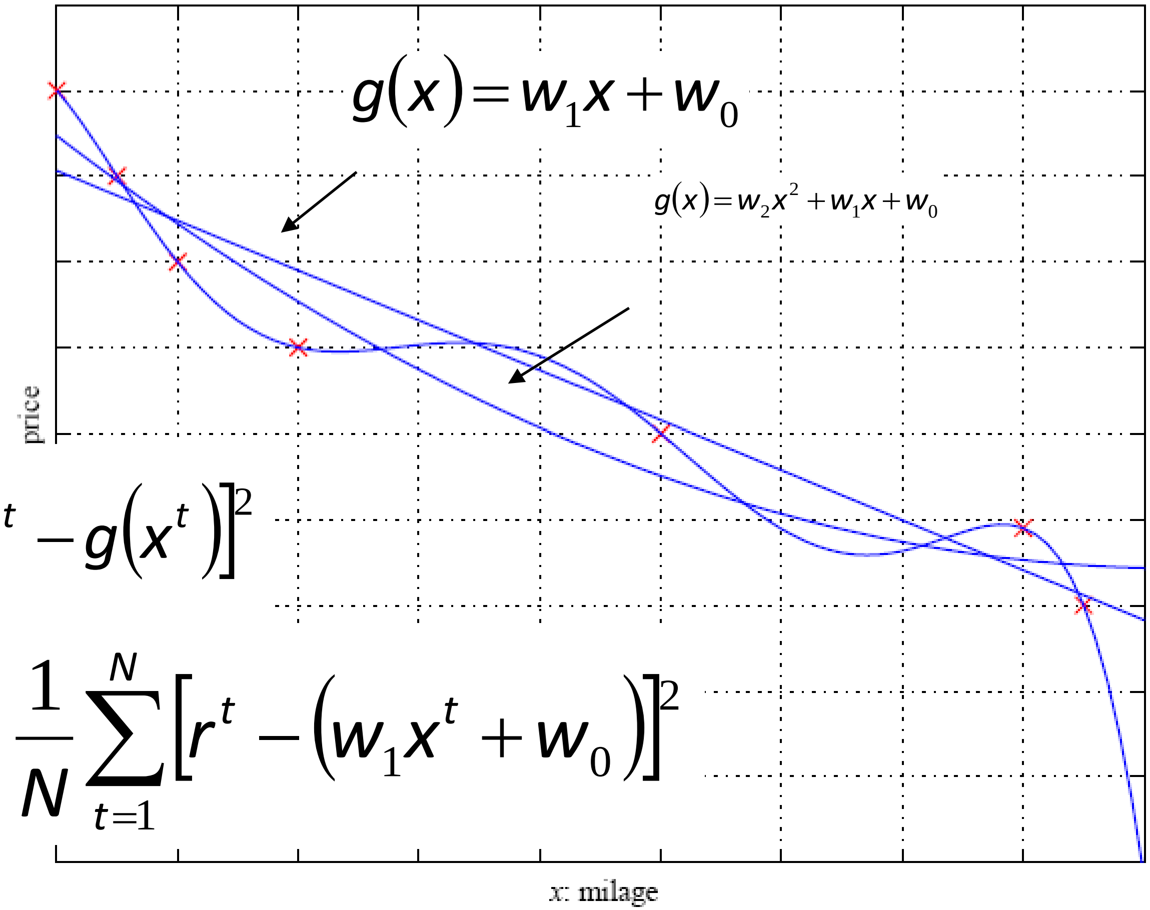
$$h_i(\mathbf{x}^t) = \begin{cases} 1 \text{ if } \mathbf{x}^t \in C_i \\ 0 \text{ if } \mathbf{x}^t \in C_j, j \neq i \end{cases}$$

Regression

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

$$r^t \in \Re$$

$$r^t = f(x^t) + \varepsilon$$



$$E(g \mid \mathcal{X}) = \frac{1}{N} \sum_{t=1}^{N} \left[r^t - g(x^t) \right]^2$$

$$E(w_1, w_0 \mid \mathcal{X}) = \frac{1}{N} \sum_{t=1}^{N} \left[r^t - (w_1 x^t + w_0) \right]^2$$

Model Selection & Generalization

- Learning is an ill-posed problem; data is not sufficient to find a unique solution
- The need for inductive bias, assumptions about $\mathcal{H}$
- Generalization: How well a model performs on new data
- Overfitting: $\mathcal{H}$ more complex than C or f
- Underfitting: $\mathcal{H}$ less complex than C or f

Triple Trade-Off

- There is a trade-off between three factors (Dietterich, 2003):
  1. Complexity of $\mathcal{H}$, c ($\mathcal{H}$),
  2. Training set size, N,
  3. Generalization error, E, on new data
- As $N\uparrow$, $E\downarrow$
- As c ($\mathcal{H}$)$\uparrow$, first $E\downarrow$ and then $E\uparrow$

Cross-Validation

- To estimate generalization error, we need data unseen during training. We split the data as
  - Training set (50%)
  - Validation set (25%)
  - Test (publication) set (25%)
- Resampling when there is few data

Dimensions of a Supervised Learner

1. Model: $g(\mathbf{x} \mid \theta)$

2. Loss function: $E(\theta \mid \mathcal{X}) = \sum_t L\left(r^t, g\left(\mathbf{x}^t \mid \theta\right)\right)$

3. Optimization procedure:

$$\theta^* = \arg\min_\theta E(\theta \mid \mathcal{X})$$