CHAPTER 2:

SUPERVISED LEARNING

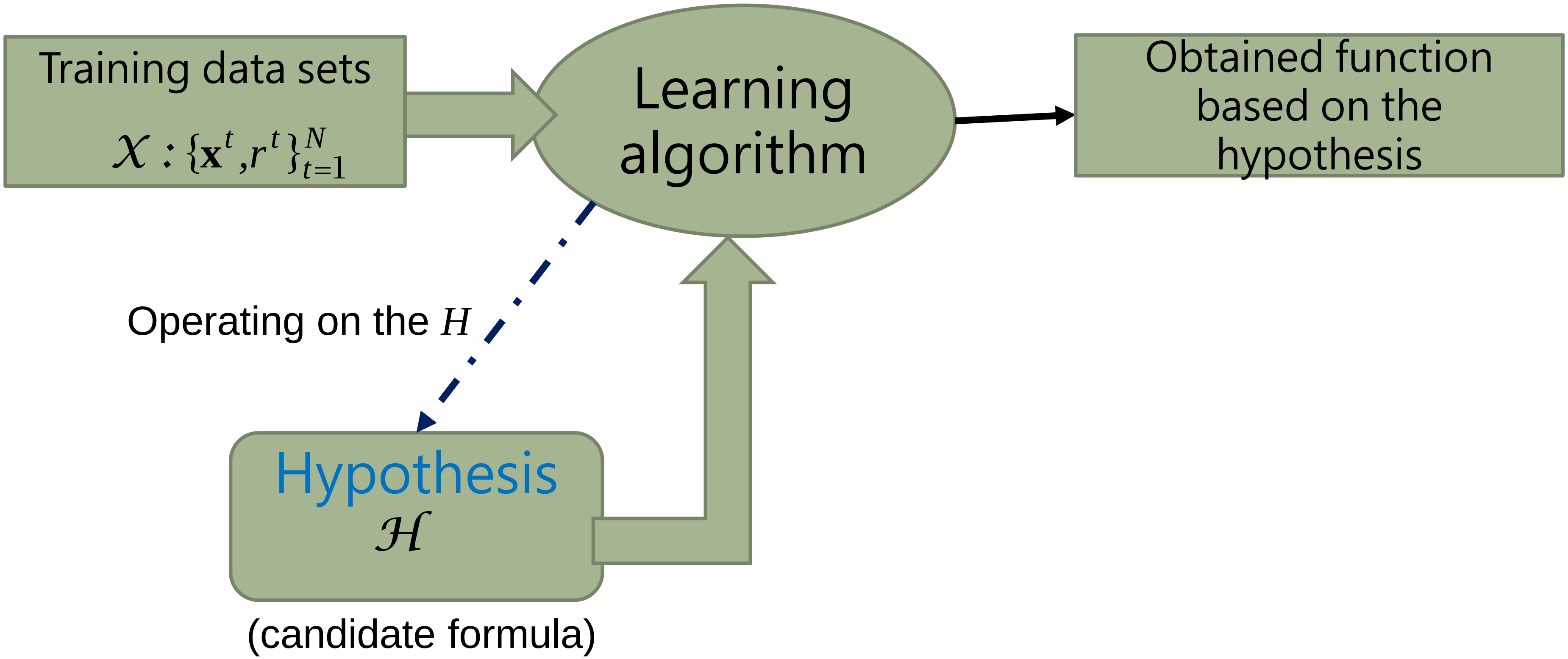
國立雲林科技大學 資訊工程研究所
張傳育(Chuan-Yu Chang) 博士
Office: EB 212
TEL: 05-5342601 ext. 4516
E-mail: chuany @yuntech.edu.tw
Website: http://MIPL.yuntech.edu.tw

Supervised vs Unsupervised learning

- Supervised learning:
  - Target of training for each training datum is provided
  - Usually the target is used to build cost function
  - Equations are derived to minimize the cost function
  - E.g. Classification,

- Unsupervised learning
  - No target is provided
  - A specific rule of updating is used but no target is provided
  - Equations are derived from the patterns for optimization
  - E.g. clustering

How machine learns?



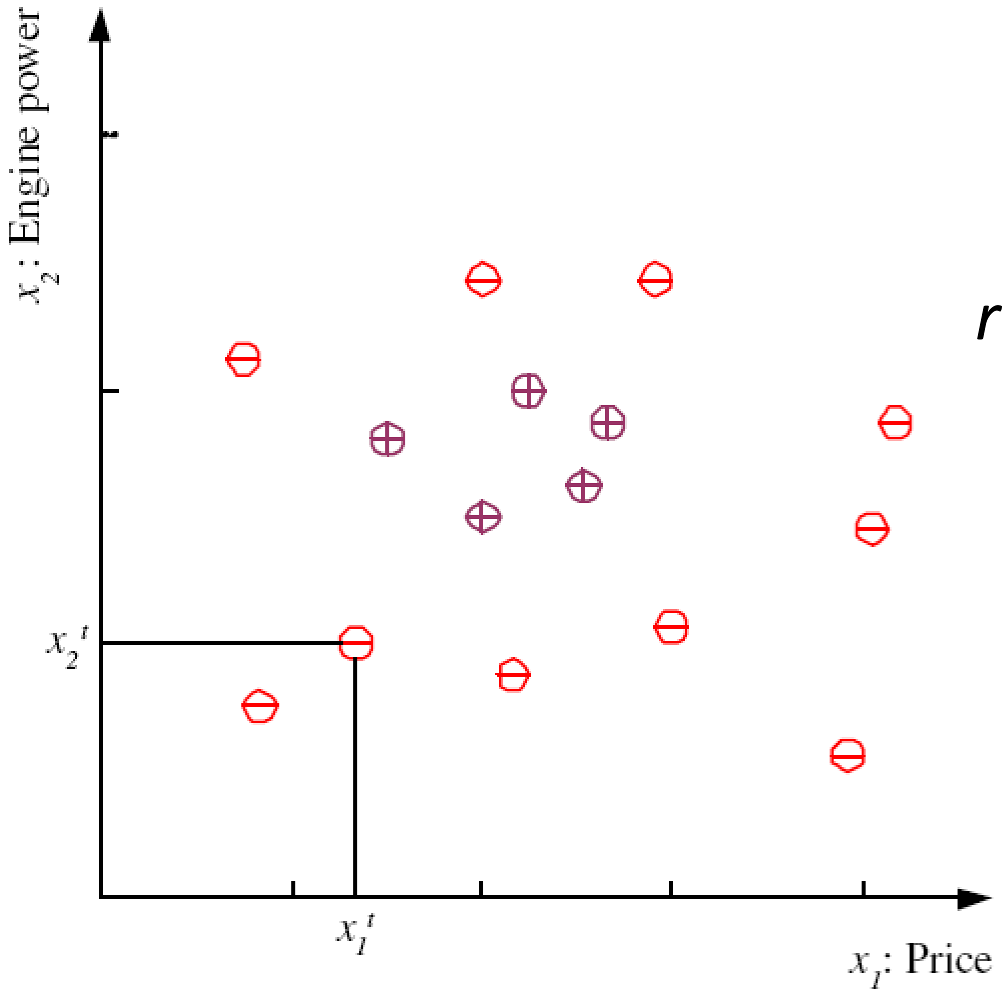
Learning a Class from Examples

- 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 $\mathcal{X}$



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

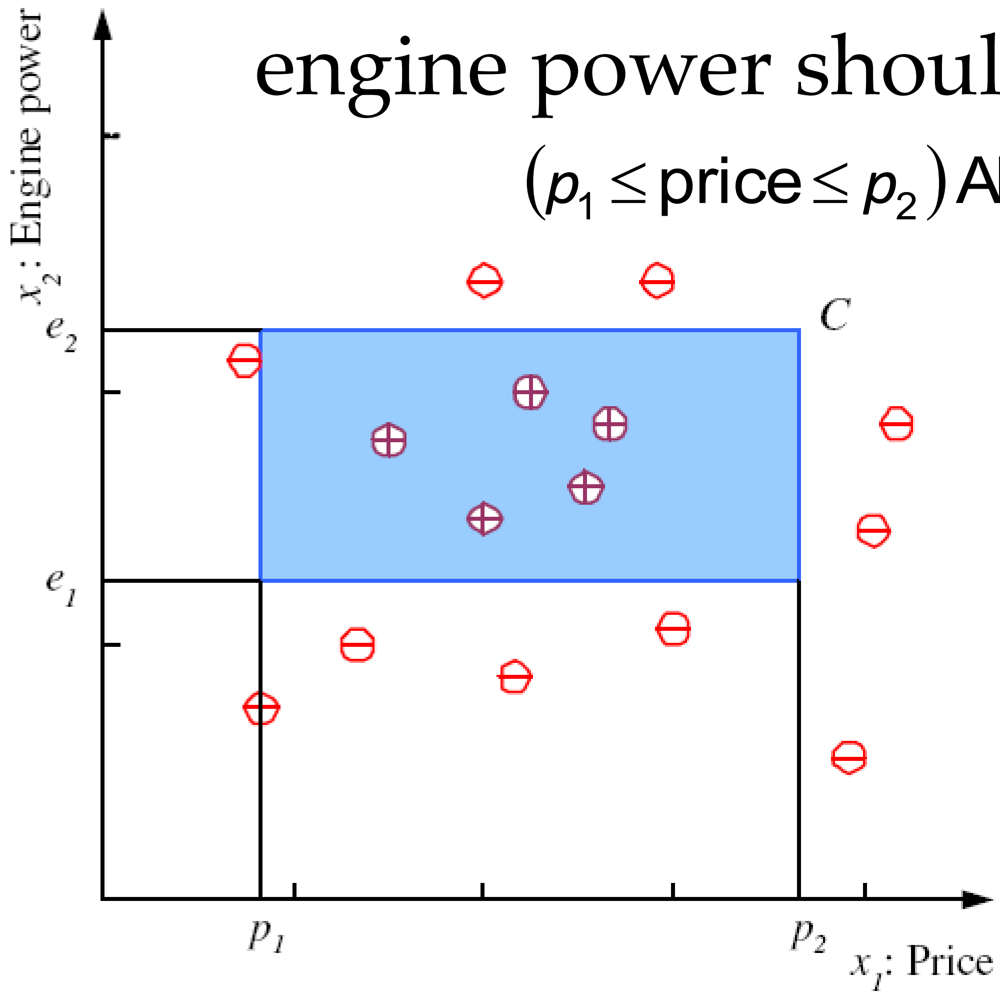
$$r = \begin{cases} 1 \text{ if } \mathbf{x} \text{ is positive} \\ 0 \text{ if } \mathbf{x} \text{ is negative} \end{cases}$$

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

Class C

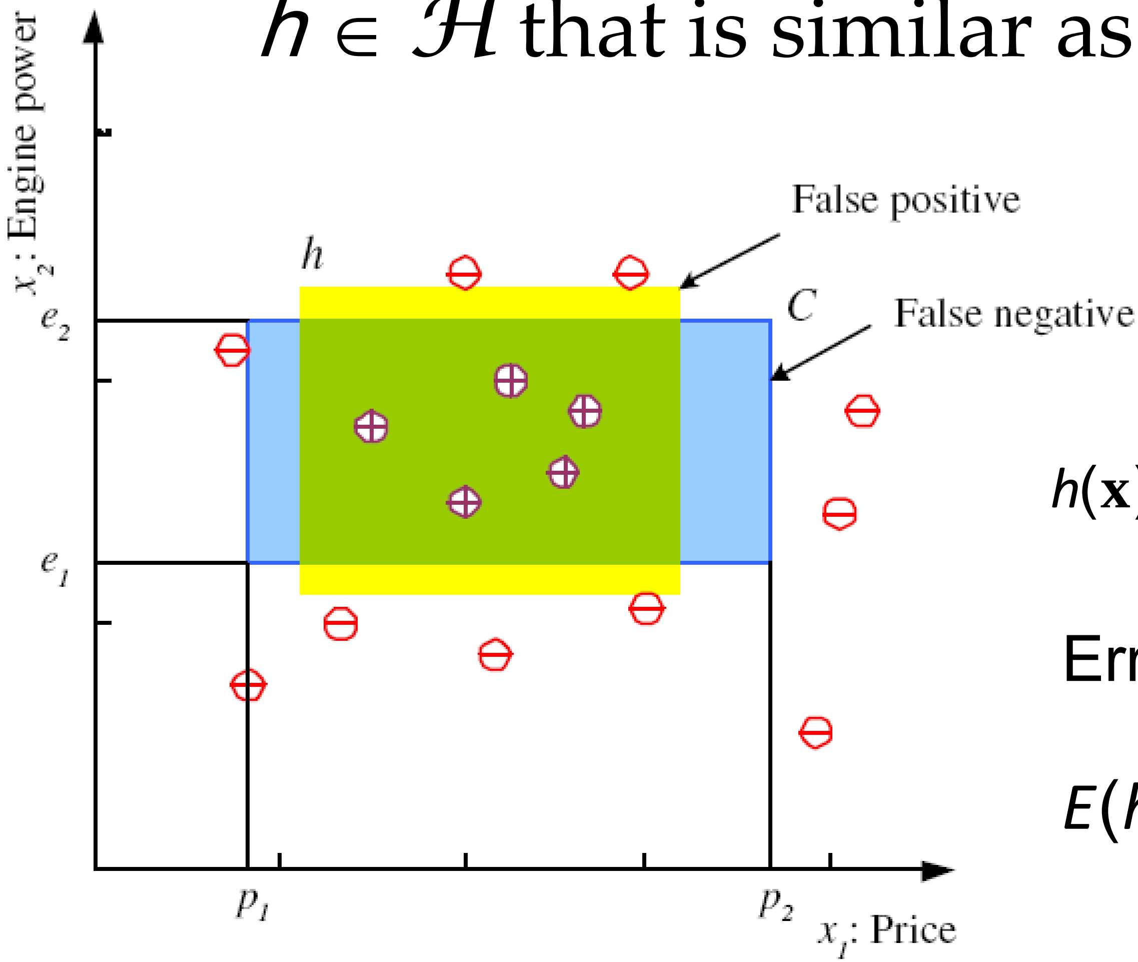
For a car to be a family car, its price and engine power should be in a certain range

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



Hypothesis class $\mathcal{H}$

The aim of learning algorithm is to find $h \in \mathcal{H}$ that is similar as possible to C.



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

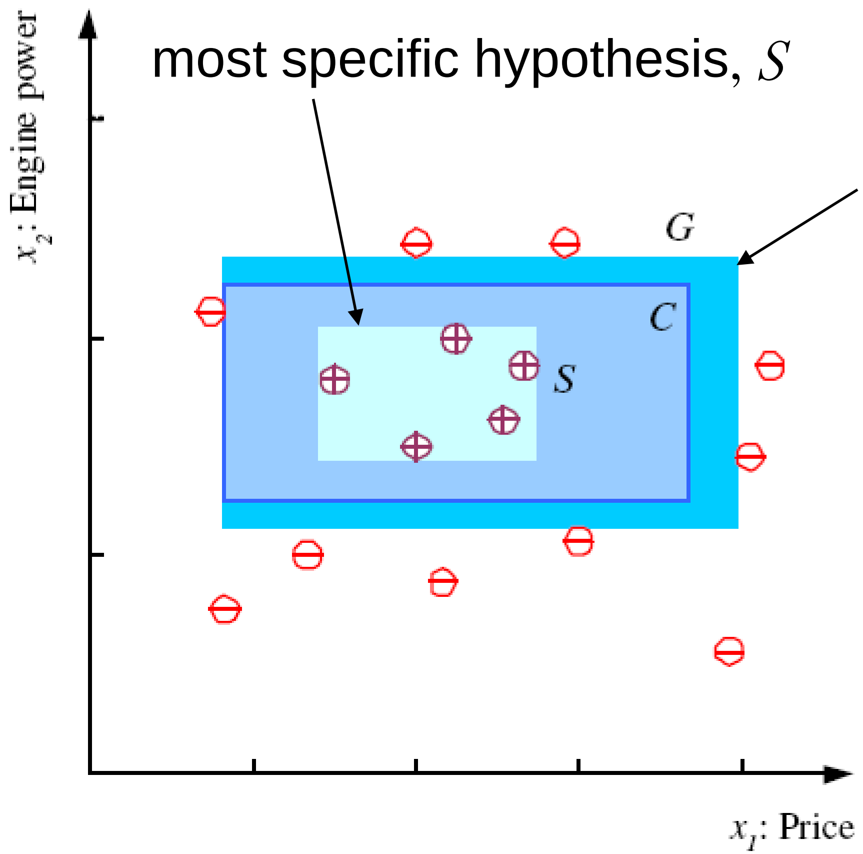
Error of h on $\mathcal{H}$

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

Generalization

- Generalization
  - How well the hypothesis will correctly classify future examples that are not part of the training set.
- To find the most specific hypothesis, S, that is the tightest rectangle that includes all the positive examples and none of the negative examples.
- The most general hypothesis, G, is the largest rectangle we can draw that includes all the positive examples and none of the negative examples.

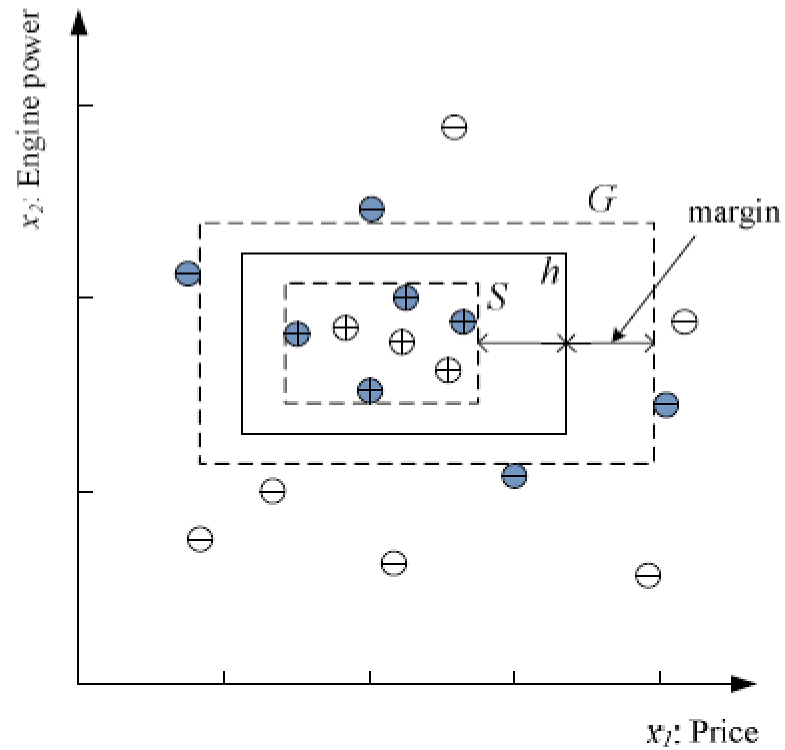
S, G, and the Version Space



Any h $\in \mathcal{H}$, between S and *G* is a valid hypothesis with no error, said to be consistent with the training set, and such *h* make up the version space (Mitchell, 1997)

Margin

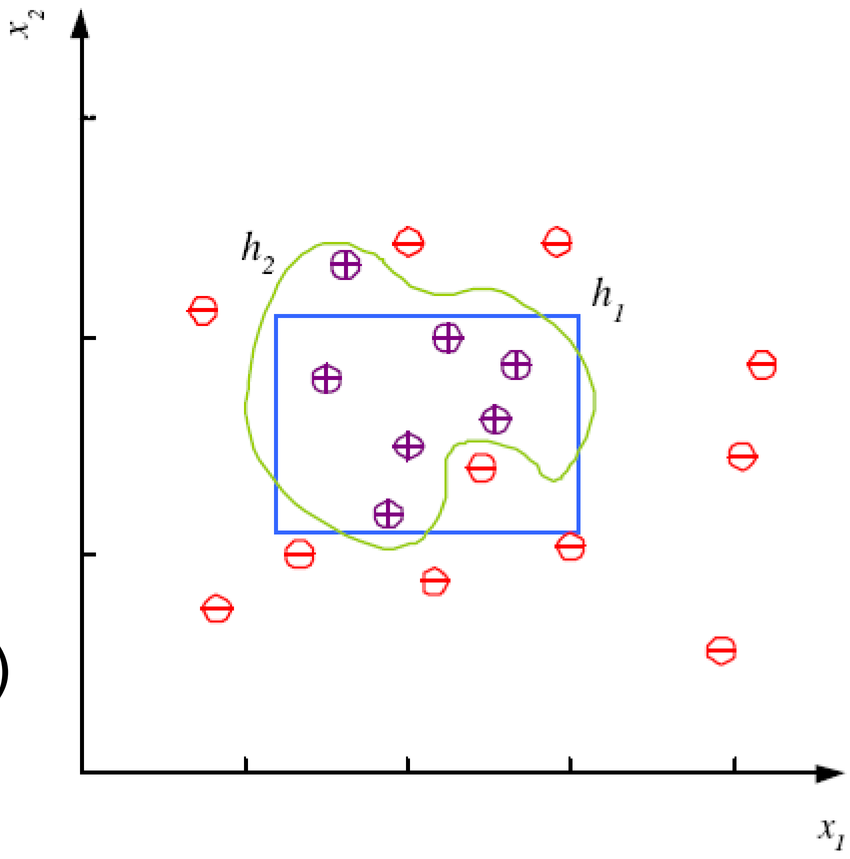
- Choose h with largest margin and minimum error function.
  - Any instance that falls in between S and G is a case of doubt, which we cannot label with certainty due to lack of data.
  - The system rejects the instance and defers the decision to a human expert.



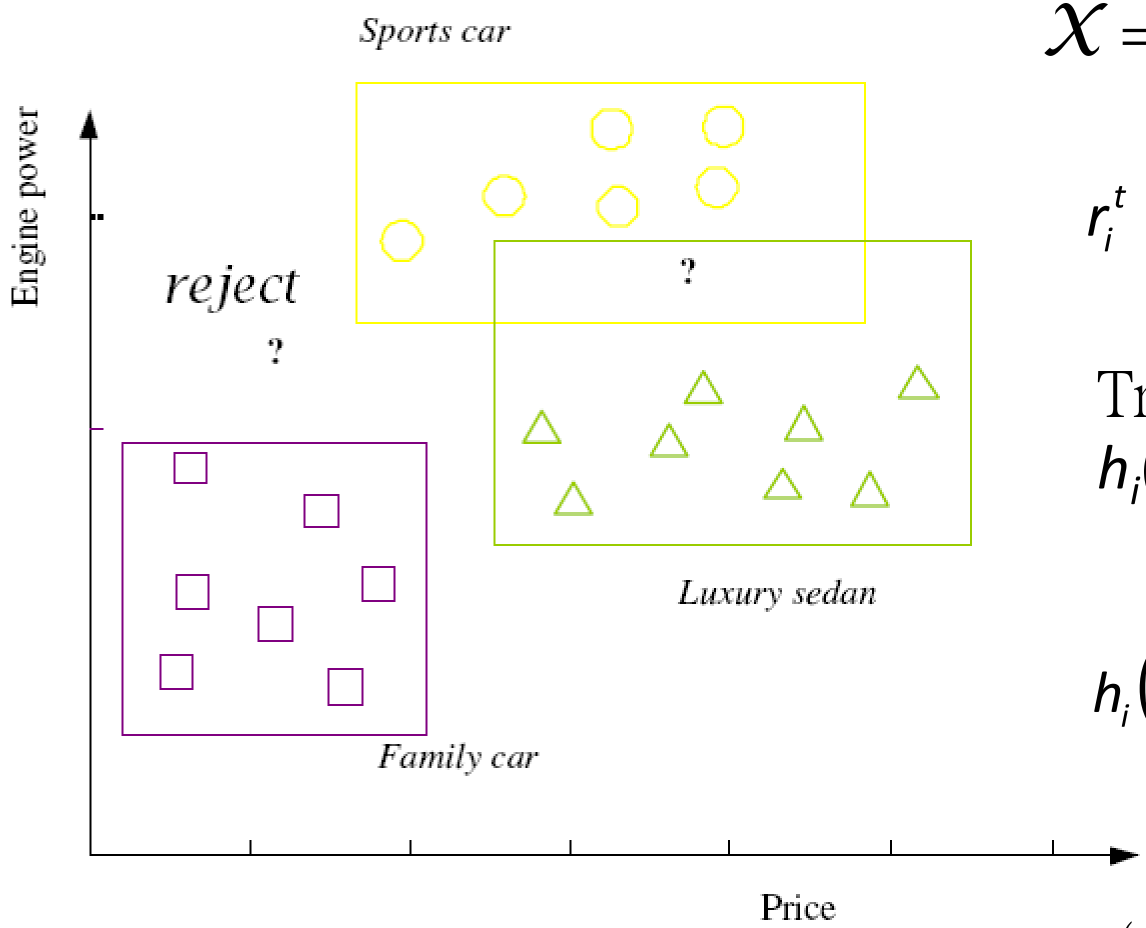
Noise and Model Complexity

Use the simpler hypothesis 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
$h_i(\mathbf{x})$, i =1,...,K:

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

$$E(\{h_i\}_{i=1}^k \mid \mathcal{X}) = \sum_{t=1}^N \sum_{i=1}^K 1(h_i(x^t) \neq r_i^t)$$

Regression

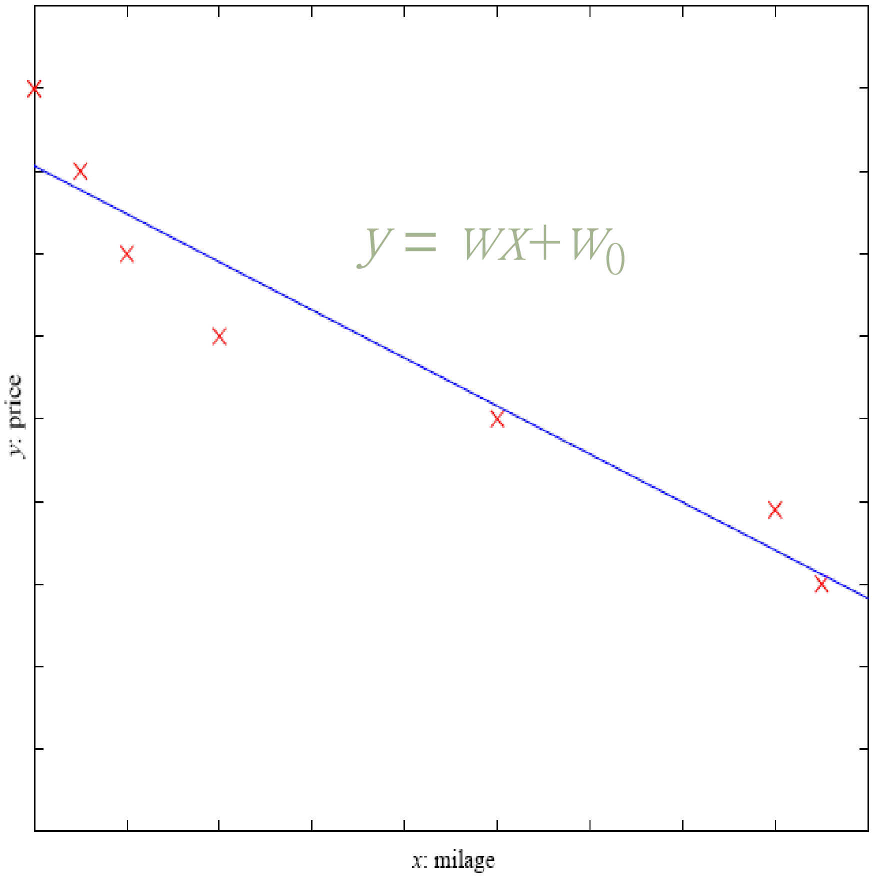
- Example: Price of a used car
- x : car attributes

  y : price

  $$y = g(x \mid \theta)$$

  $g(.)$: model,

  θ : parameters

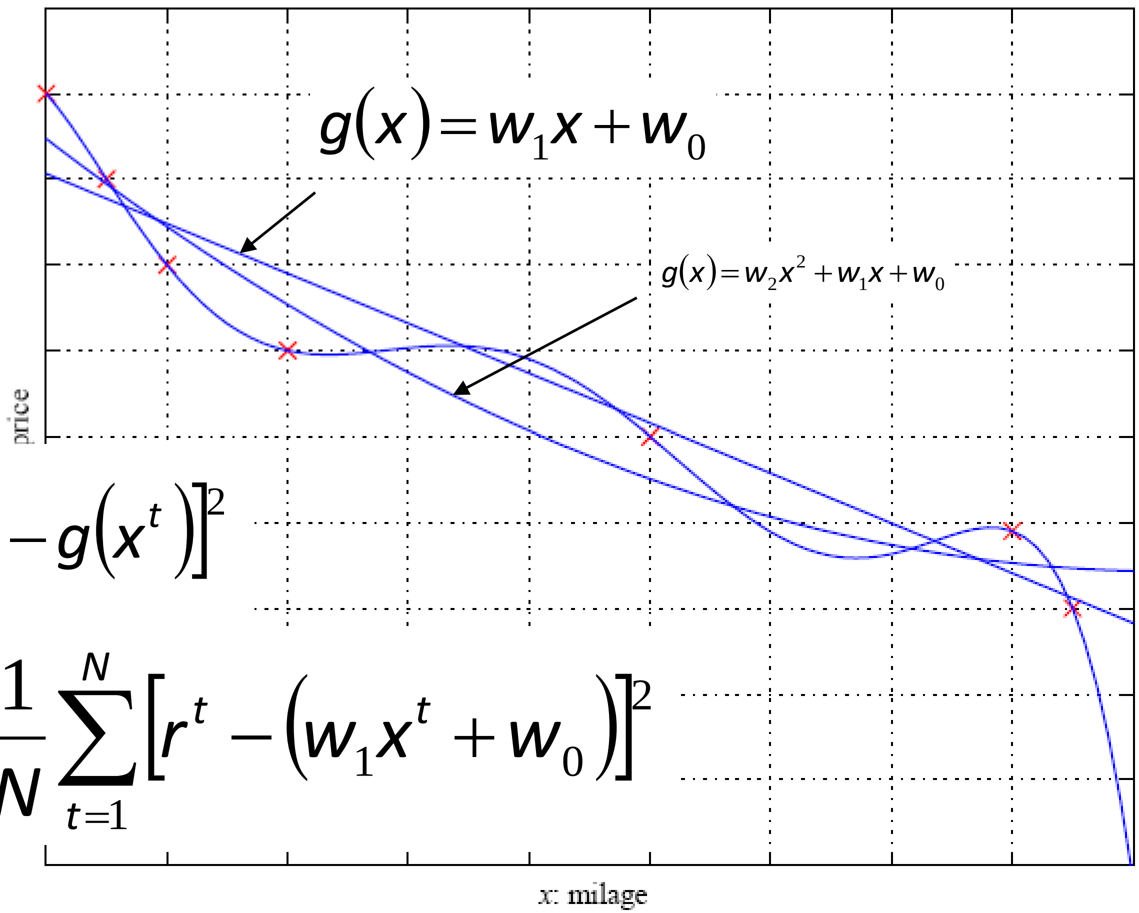


Regression

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

$$r^t \in \Re$$

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



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

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

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

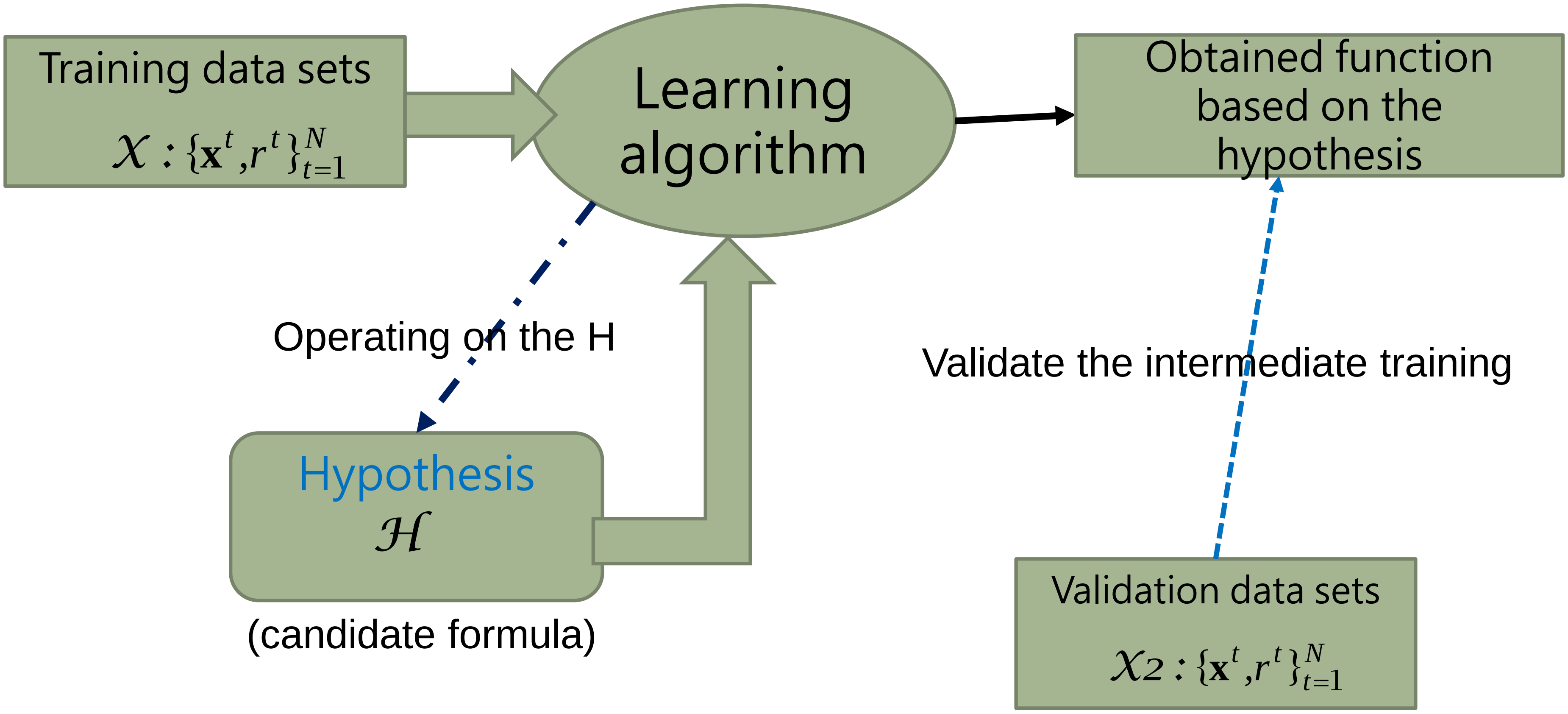
Triple Trade-Off

- 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

Cross validation



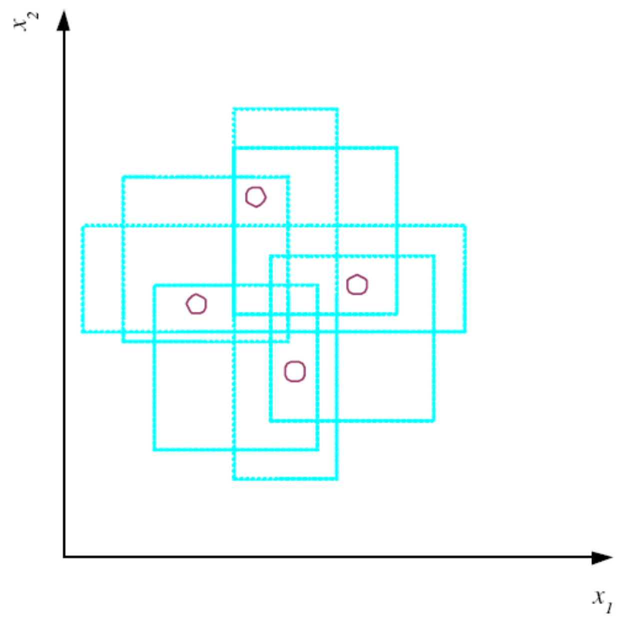
Dimensions of a Supervised Learner

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:

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

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: 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 $N \geq (4/\varepsilon)\log(4/\delta)$