Machine Learning Basics

Announcements:

1. Warmup Quiz and P(-1) and P(0) are out

2. TA office hours are posted on Canvas (location: Rhodes 503)

3. CIS Partner Finding Social (Sep 1st, 4-6pm, Upson 142)

Objective:

Get familiar with some of the common definitions, and get a big picture of supervised / unsupervised learning

Outline for Today:

1. Supervised Learning (Classification / Regression) and Unsupervised learning

2. Generalization

3. Training / validation / testing

Classification

Dataset $\mathscr{D}$

( ,cat) ( ,cat) ( ,dog)

Classification

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ML model

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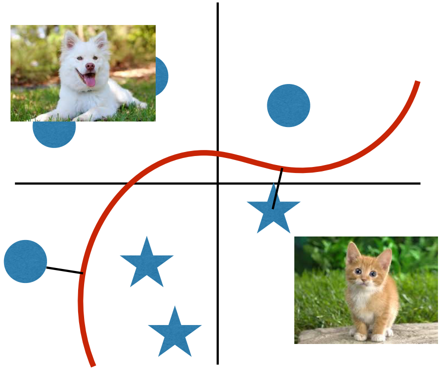

Mathematical formulation of the pipeline

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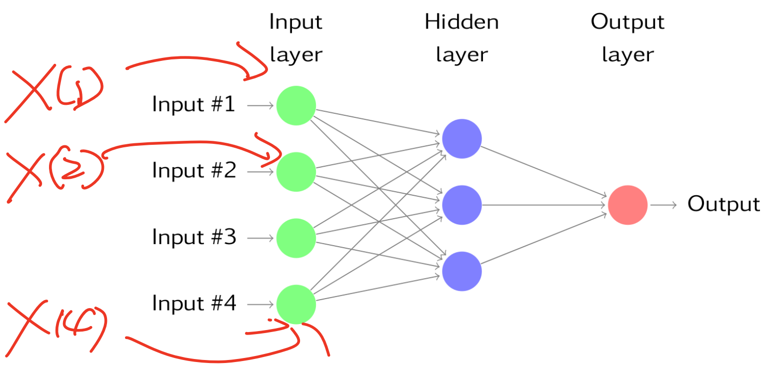

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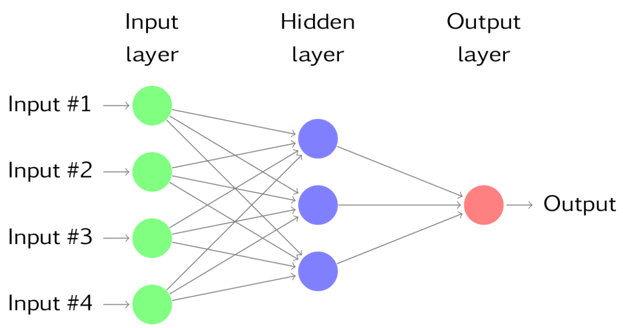

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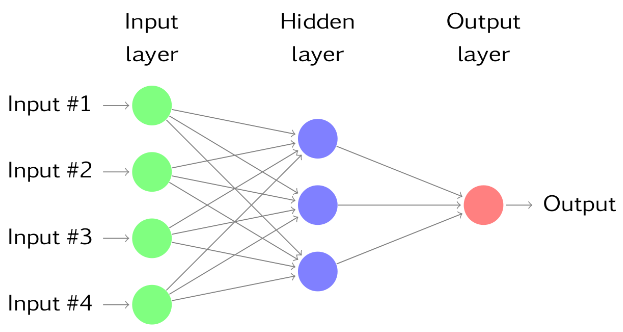

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i.e., a large family of NNs with different parameters

Examples of hypothesis

Inductive bias (i.e., assumptions) encoded in the hypothesis class

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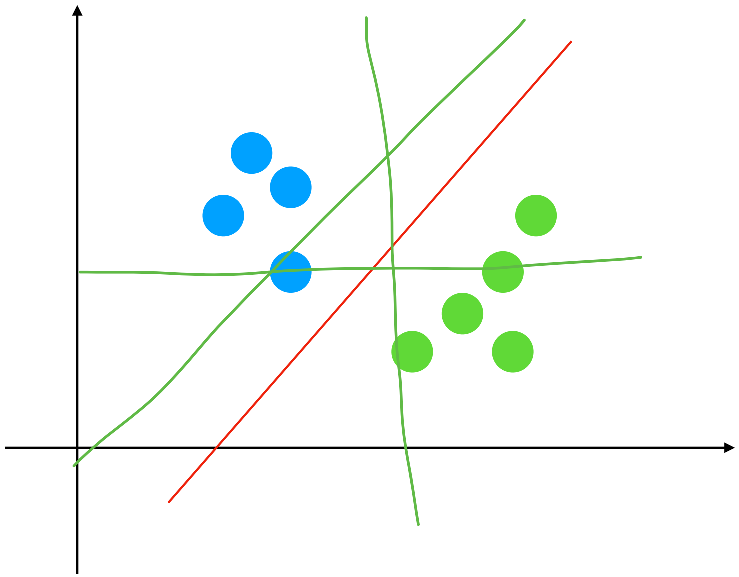
$\mathscr{H}$ contains all possible linear functions



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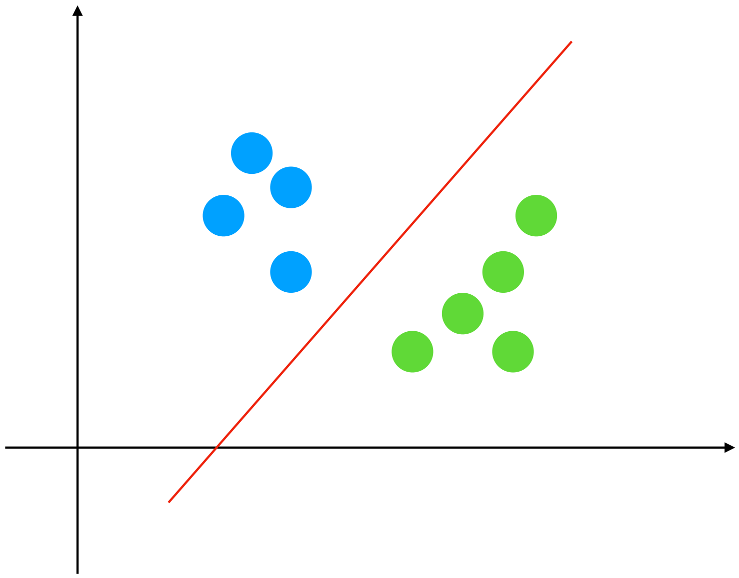
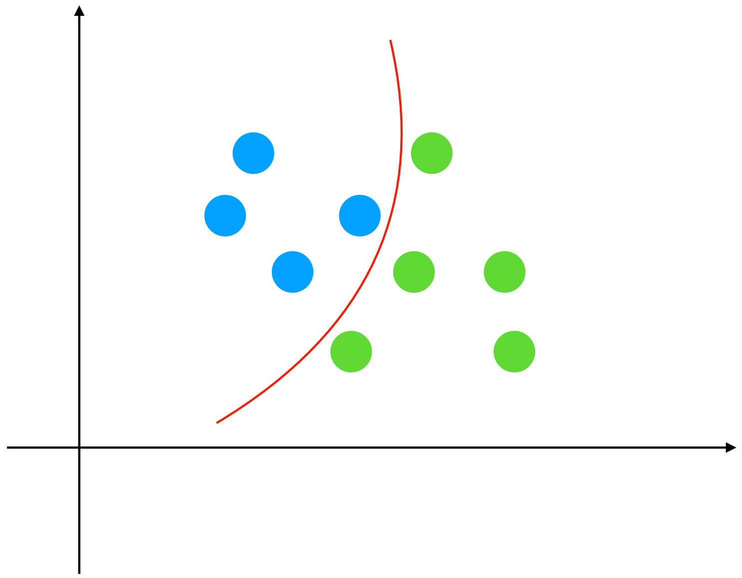


Ex: h is nonlinear $h(x) = \mathrm{sign}(w^\top (\mathrm{relu}(Ax)))$;
$\mathscr{H}$ contains all possible one-layer NN



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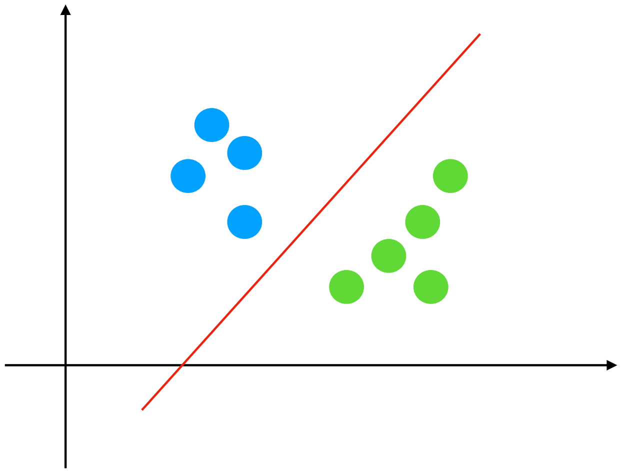

We use prior knowledge (i.e., we believe linear function is enough) to design an ML algorithm here

The Loss Function

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Zero-one loss:

$$\ell(h, x, y) = \begin{cases} 0 & h(x) = y \\ 1 & h(x) \neq y \end{cases}$$

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Squared loss:

$$\ell(h, x, y) = (h(x) - y)^2$$

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With loss ℓ being defined, we can perform training/learning:

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e.g., total number of mistakes h makes on n training samples (training error)

Putting things together: Binary classification

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( ,cat) ( ,cat) ( ,dog)

x_1, y_1 x_2, y_2 x_3, y_3

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ML model, e.g., neural network w/ 0-1 loss

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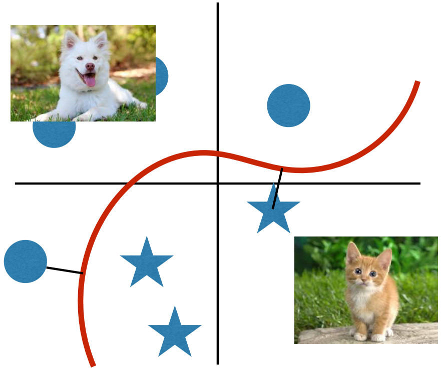

Regression

Example: learning to drive from expert

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Training: minimizing mean squared error (MSE)

$$\arg\min_{\theta} \sum_i (\theta^\top x_i - y_i)^2$$

Application of Regression: training self-driving cars *[Pomerleau, NeurIPS '88]*

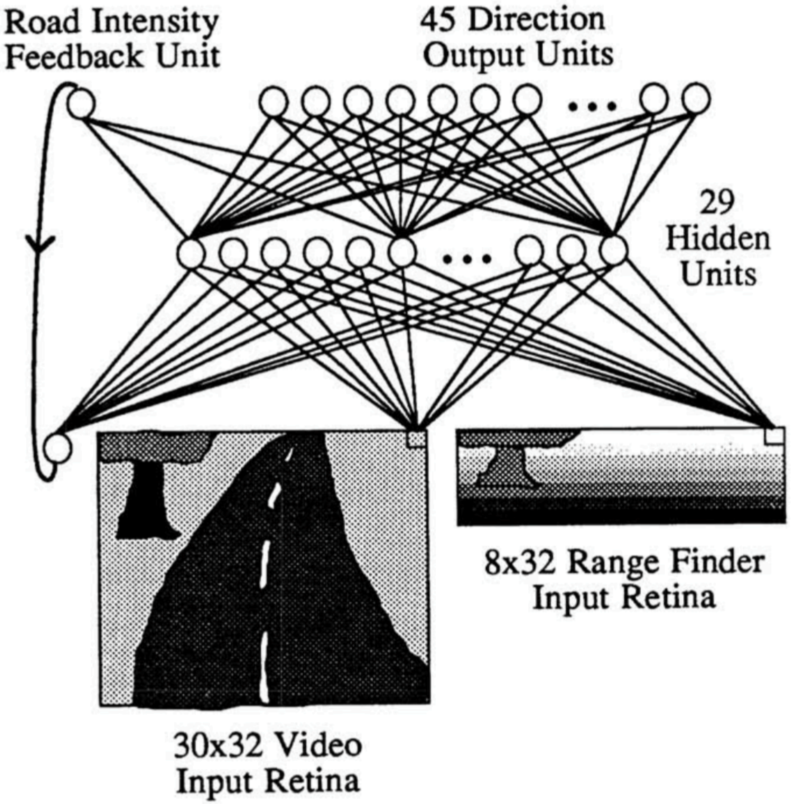

Figure 1: ALVINN Architecture

Unsupervised Learning

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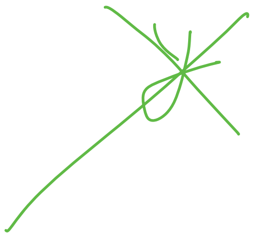

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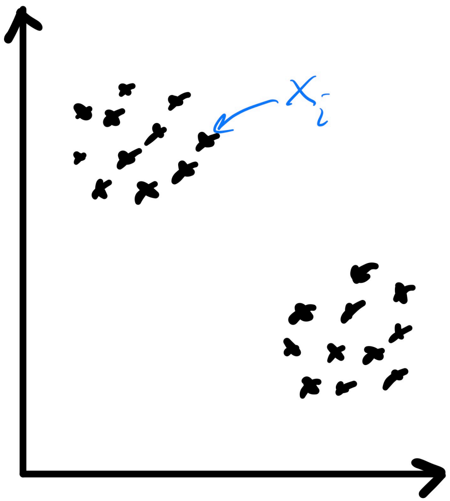

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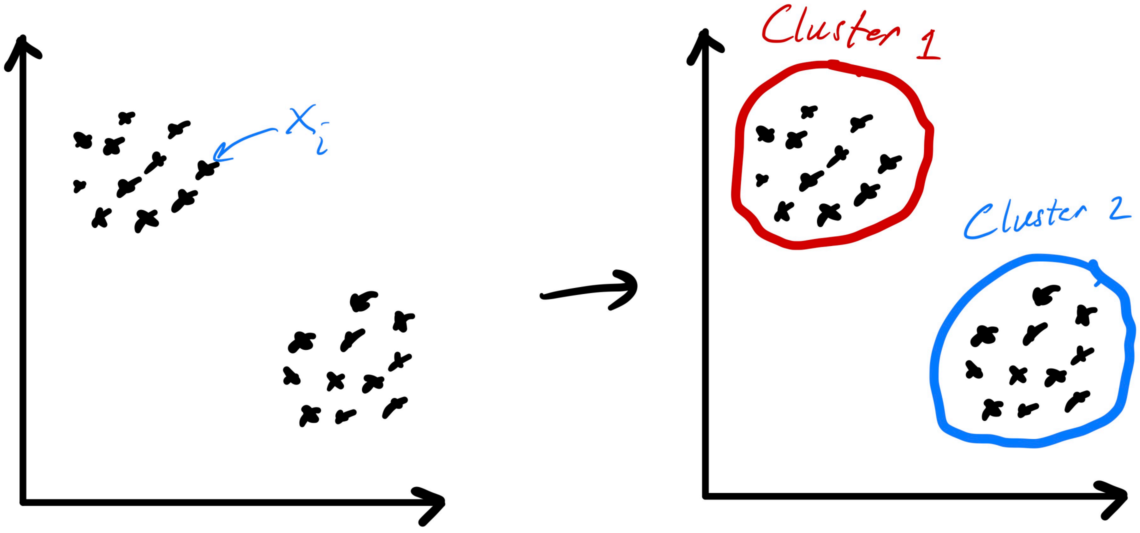

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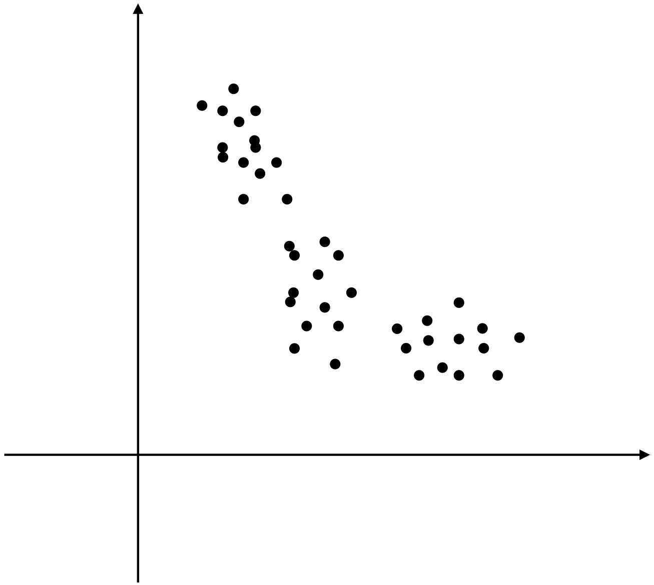

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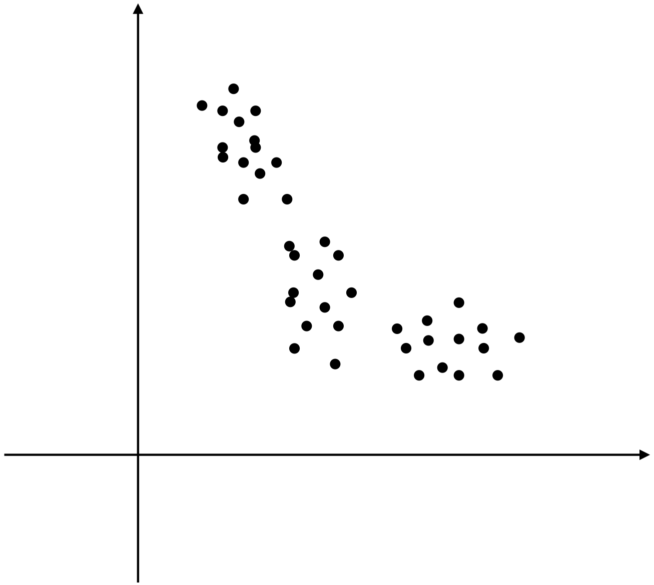

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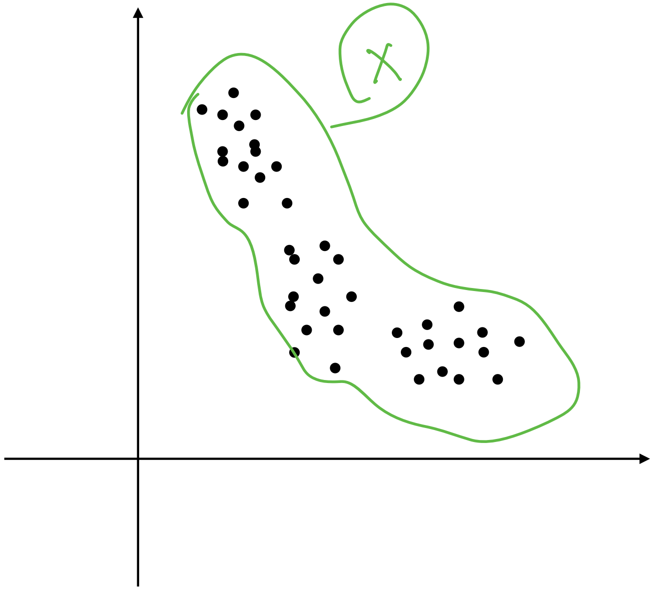

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Anomaly detection / generative AI

Application of distribution estimation: face generator

Generated images:

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Similar images from the dataset

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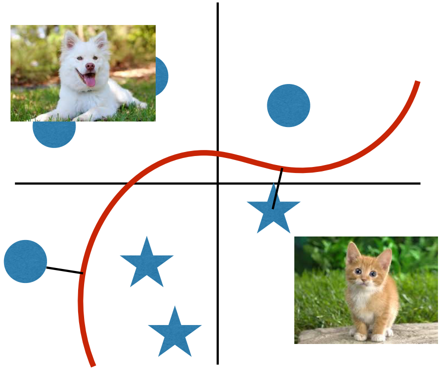

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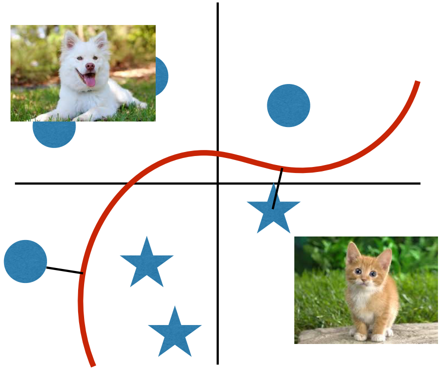

Generalization: how well can our trained model do on <u>unseen test examples</u>?

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e.g., expected classification error of $\hat{h}$

Overfitting

Overfitting: we have a small training error but large generalization error

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Example

Hypothesis $\tilde{h}$ that **memorizes** the whole training set

$$\tilde{h}(x) = \begin{cases} y_i & \exists (x_i, y_i) \in \mathscr{D} \text{ w/ } x_i = x \\ -1 & \text{else} \end{cases}$$

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What is the training error? Is this a good classifier?

Traing Err = $\sum_{i=1}^{n} \mathbb{1}(\tilde{h}(x_i) \neq y_i)$

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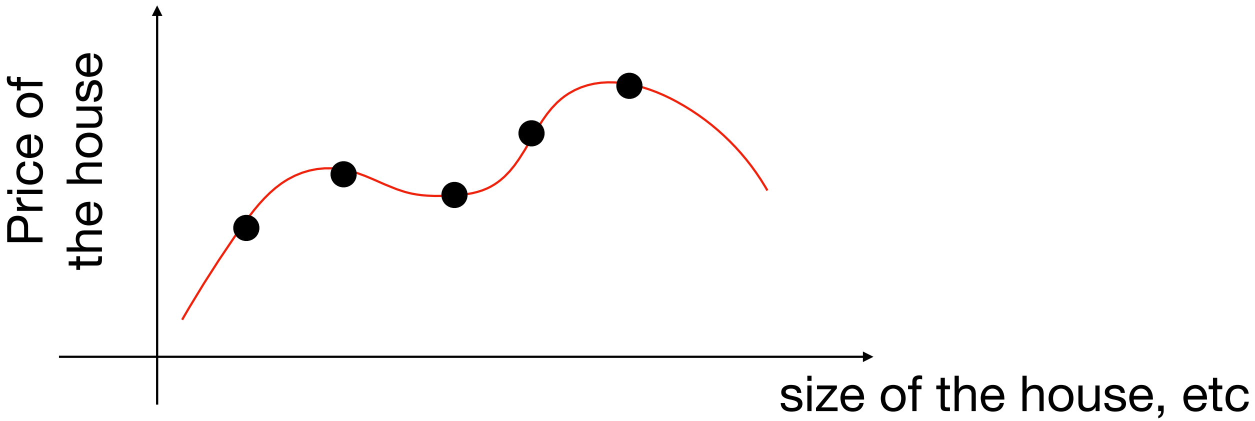

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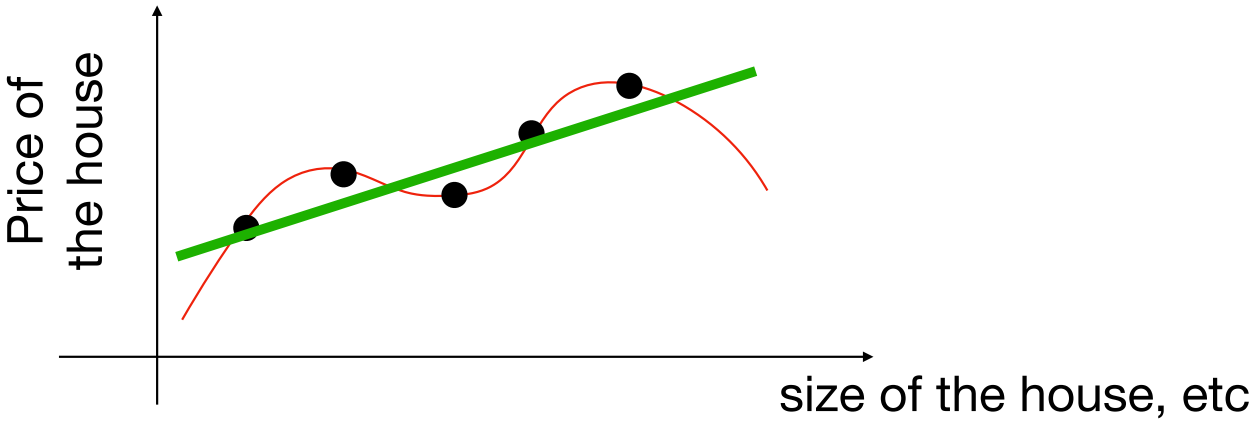

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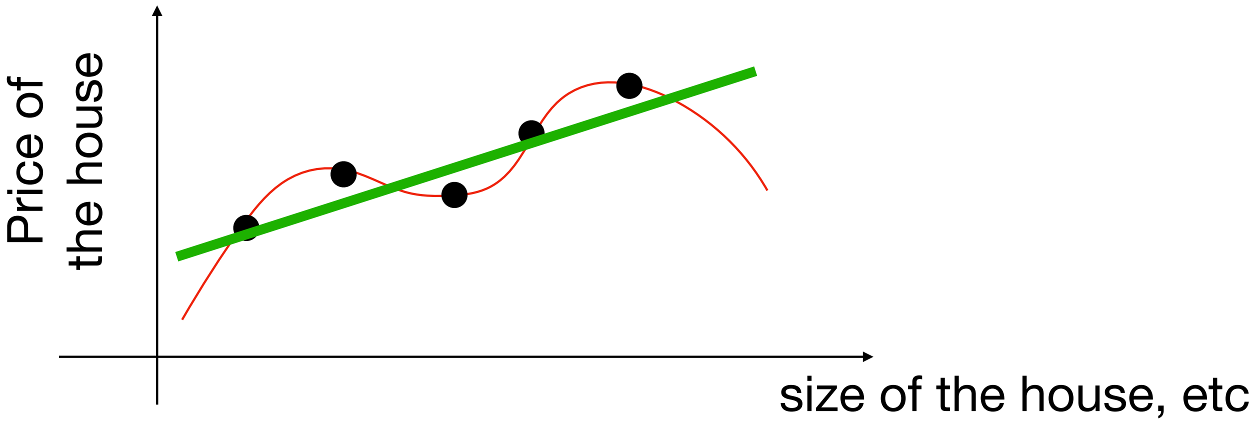

Training error = 0 (e.g., we probably overfit to noises), but could do terribly on test examples

Overfitting

How to tell that our models overfit?

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Training, validation, and testing

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$\mathscr{D}_{TR}$: training set

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Before training/learning, we often **randomly** split it with size proportional to 80% / 10% / 10%

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Revise model on $\mathscr{D}_{TR}$ (e.g., add regularization, change neural network structures, etc)

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$\Downarrow \Uparrow$

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Such independence implies that:

$$\frac{1}{|\mathcal{D}_{TE}|} \sum_{x,y \in \mathcal{D}_{TE}} \ell(\hat{h}, x, y) \approx \mathbb{E}_{x,y \sim \mathcal{P}}[\ell(\hat{h}, x, y)]$$

(Due to law of large numbers)

Other ways to split the data?

Can we split data based on features, or labels?

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Often repeated many times using validation $\mathscr{D}_{VA}$

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1. Given a task and a dataset $\mathscr{D} = \{x_i, y_i\}, x_i, y_i \sim \mathscr{P}$

2. Design hypothesis class $\mathscr{H}$ and loss function ℓ (encodes inductive bias)

3. Train: $\hat{h} = \arg\min_{h \in \mathscr{H}} \sum_{(x,y \in \mathscr{D})} \ell(h, x, y)$

4. Output: $\hat{h}$ that has small generalization error $\mathbb{E}_{x,y\sim\mathscr{P}}[\ell(\hat{h}, x, y)]$

Often repeated many times using validation $\mathscr{D}_{VA}$