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

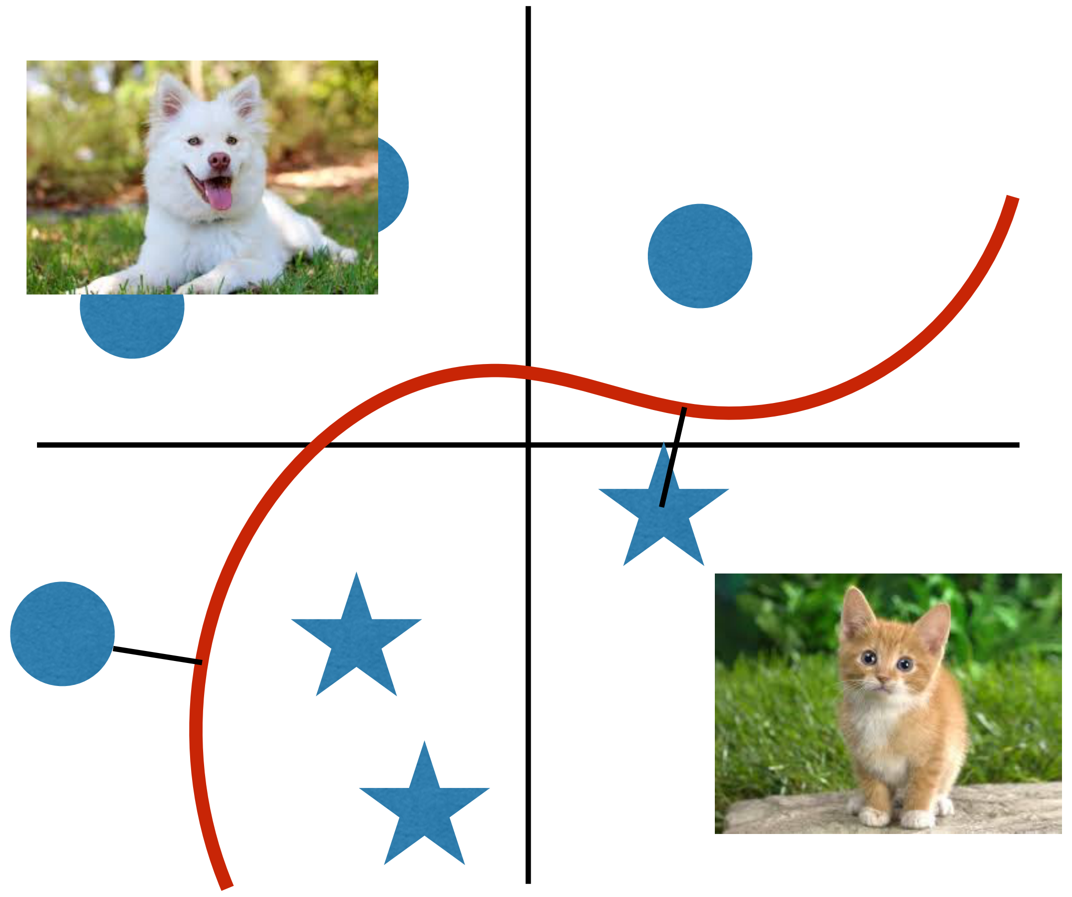
3. Training / validation / testing

Classification

Dataset $\mathscr{D}$

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

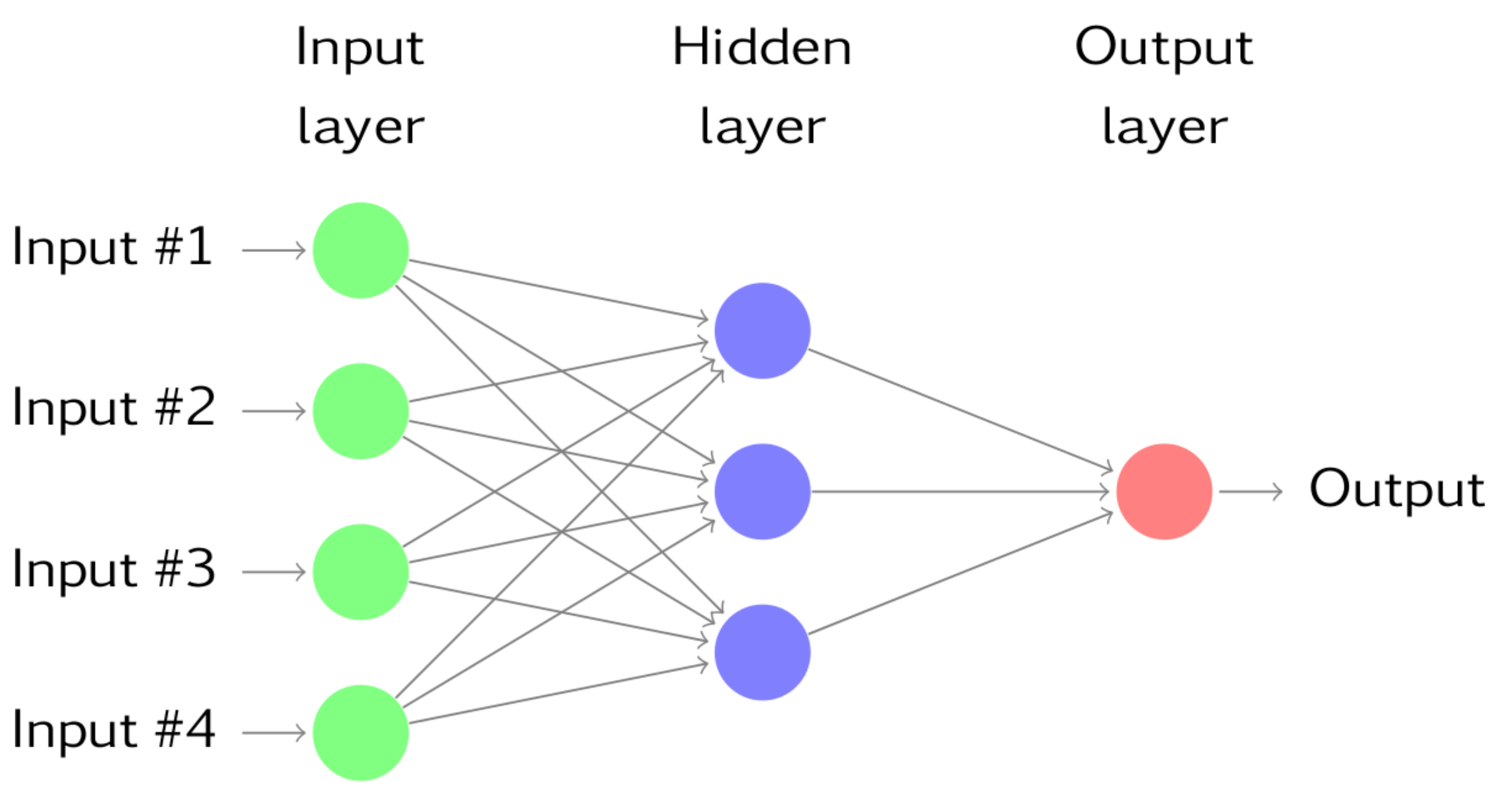
ML model



Mathematical formulation of the pipeline

Dataset:

$$\mathscr{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}, x_i \in \mathbb{R}^d, y_i \in \mathscr{C}(\text{ e.g.,} \mathscr{C} = \{-1,1\}), (x_i, y_i) \sim \mathscr{P}$$



Hypothesis:

$$h : \mathbb{R}^d \mapsto \mathscr{C}$$

i.e., a neural network-based classifier that maps image to label of cat or dog

Hypothesis class

$$\mathscr{H} = \{h\}$$

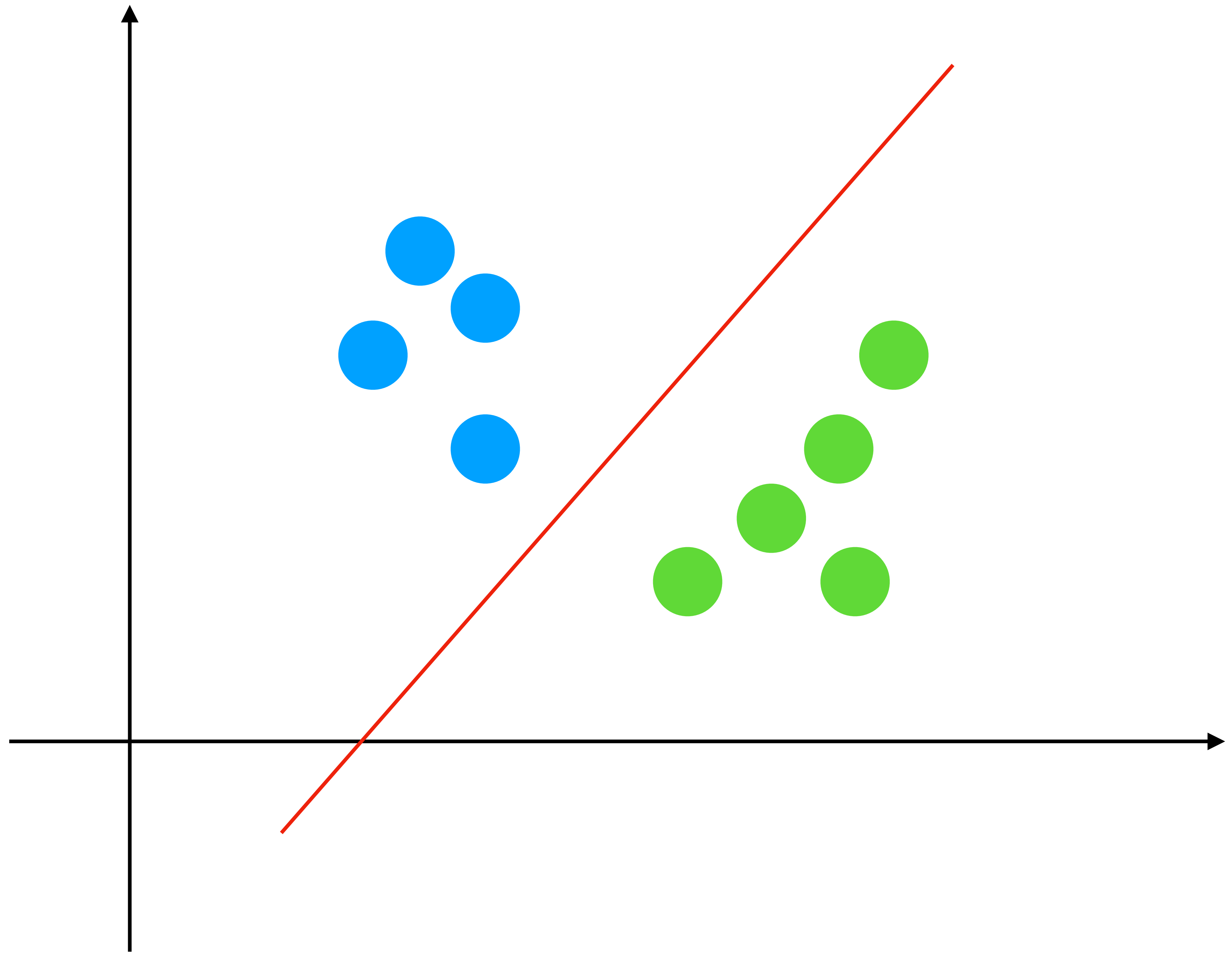
i.e., a large family of NNs with different parameters

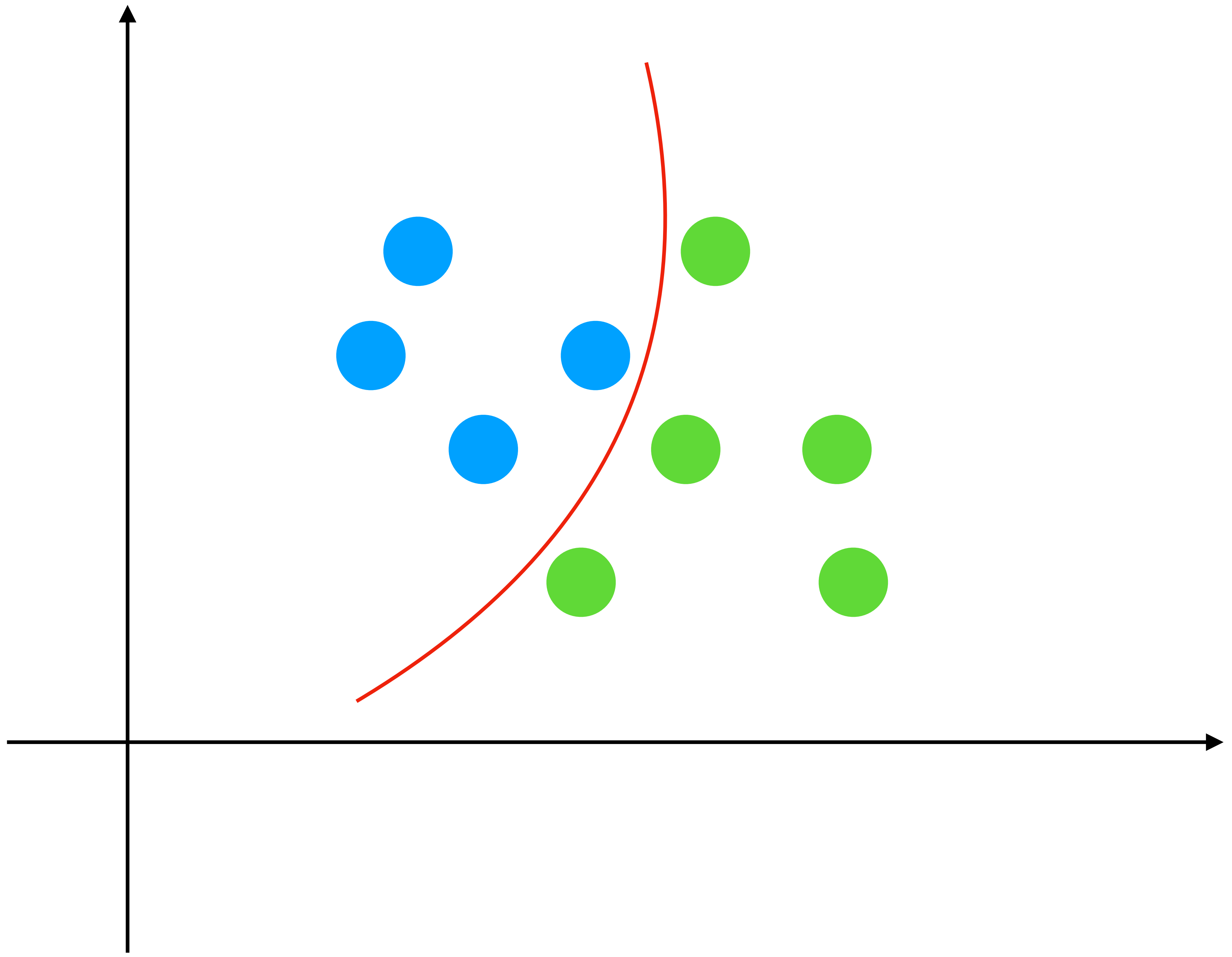
Examples of hypothesis

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

Ex: h is a linear function $h(x) = \text{sign}(w^\top x)$;
$\mathcal{H}$ contains all possible linear functions

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

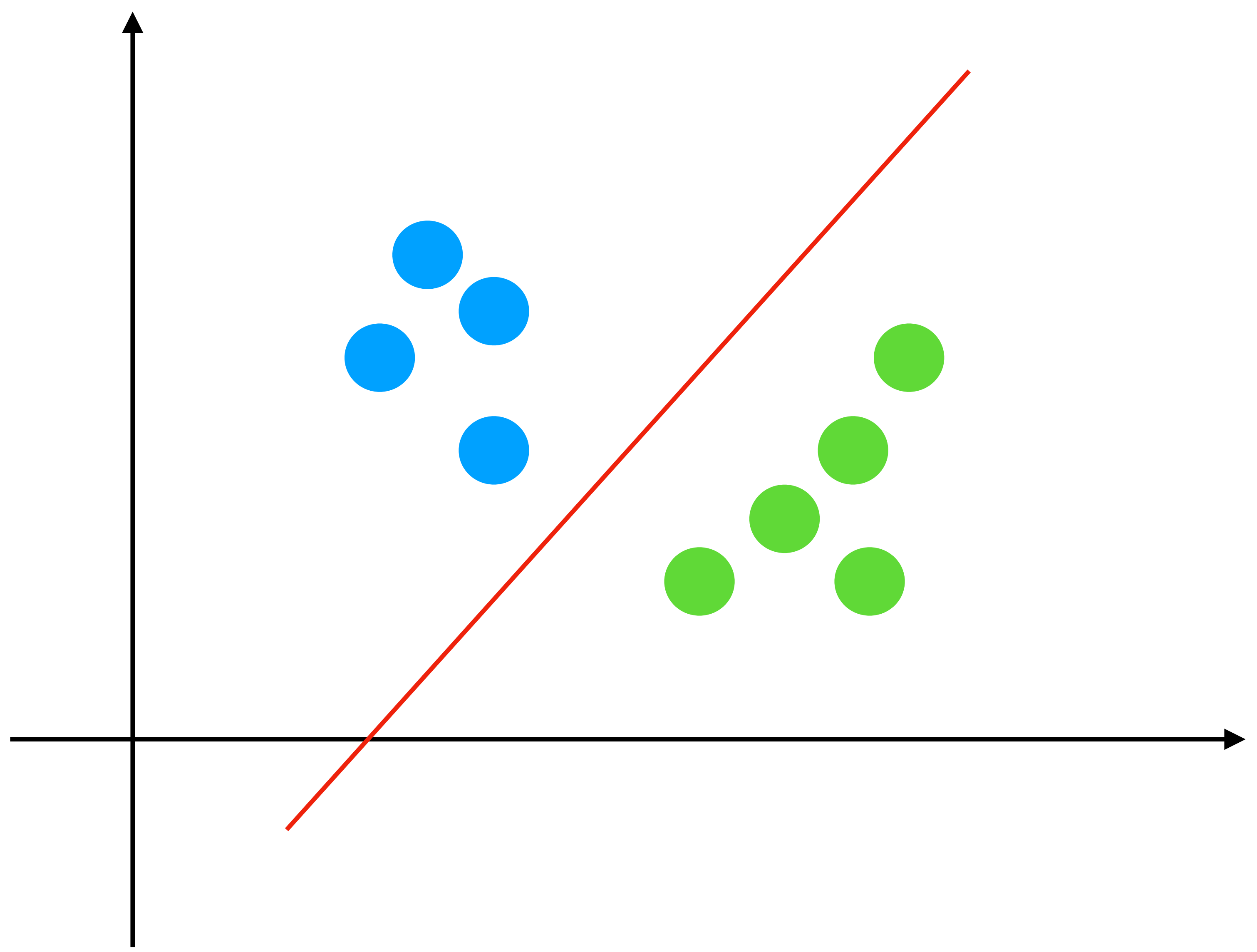




Do we need to make assumptions on the data?

No free lunch theorem says that we must make such assumptions

Informal theorem: for any machine learning algorithm $\mathscr{A}$, there must exist a task $\mathscr{P}$ on which it will fail



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

The Loss Function

Q: how to select the best hypothesis $\hat{h}$ from $\mathscr{H}$?

Let's define loss function $\ell : \mathscr{H} \times \mathbb{R}^d \times \mathscr{C} \mapsto \mathbb{R}$

Intuitively, $\ell(h, x, y)$ tells us how bad (e.g., classification mistake) the hypothesis h is.

Examples:

Zero-one loss:

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

Squared loss:

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

Learning/Training

Q: how to select the best hypothesis $\hat{h}$ from $\mathcal{H}$?

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

$$\hat{h} = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \ell(h, x_i, y_i)$$

The hypothesis that has smallest training error

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

Putting things together: Binary classification

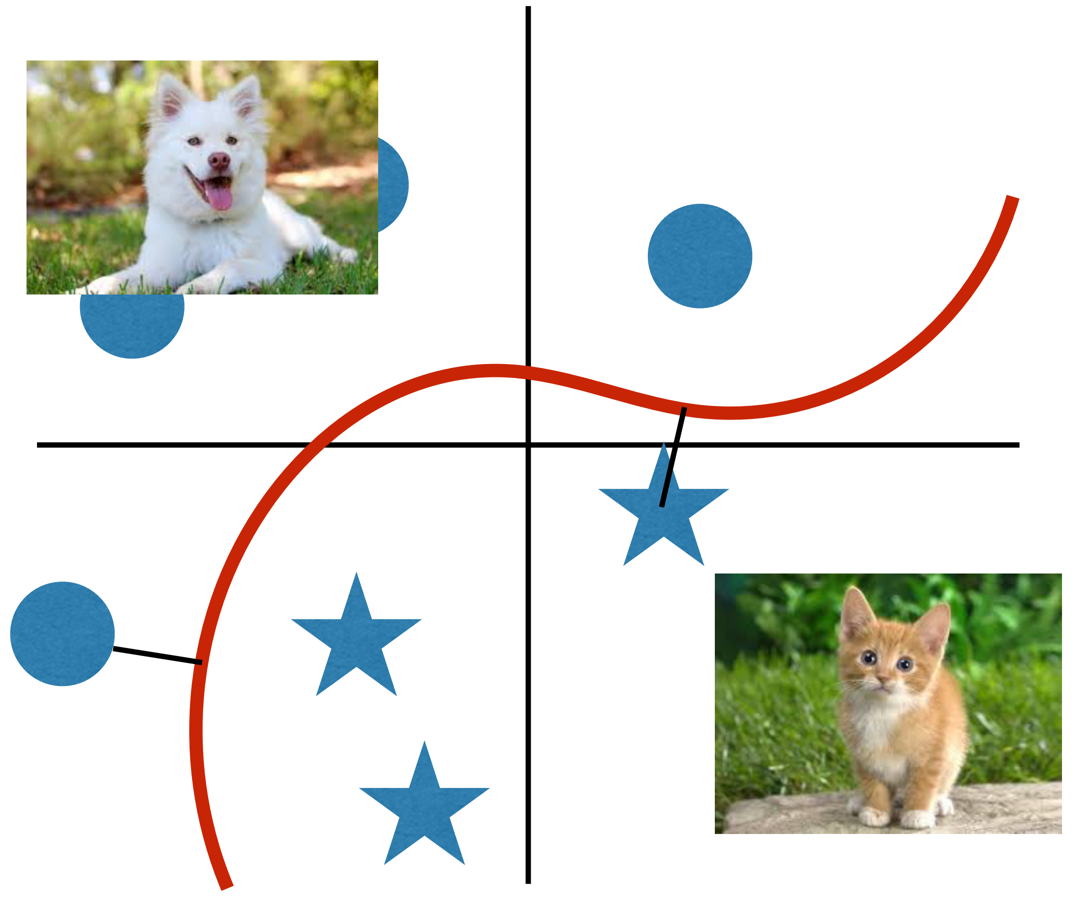
Dataset $\mathscr{D}$

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

x_1, y_1 x_2, y_2 x_3, y_3

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

$$\hat{h}_{nn} = \arg\min_{h_{nn} \in \mathscr{H}} \sum_{i=1}^{n} \ell_{0-1}\left(h_{nn}, x_i, y_i\right)$$



Regression

Example: learning to drive from expert

Feature x

Expert steering angle y

$$\mathscr{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$$

collected by human expert

Continuous variable $(-\pi, \pi)$

Loss function: square loss

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

Hypothesis class: linear functions

$$h(x) := \theta^\top x, \text{ where } \theta \in \mathbb{R}^d$$

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]*

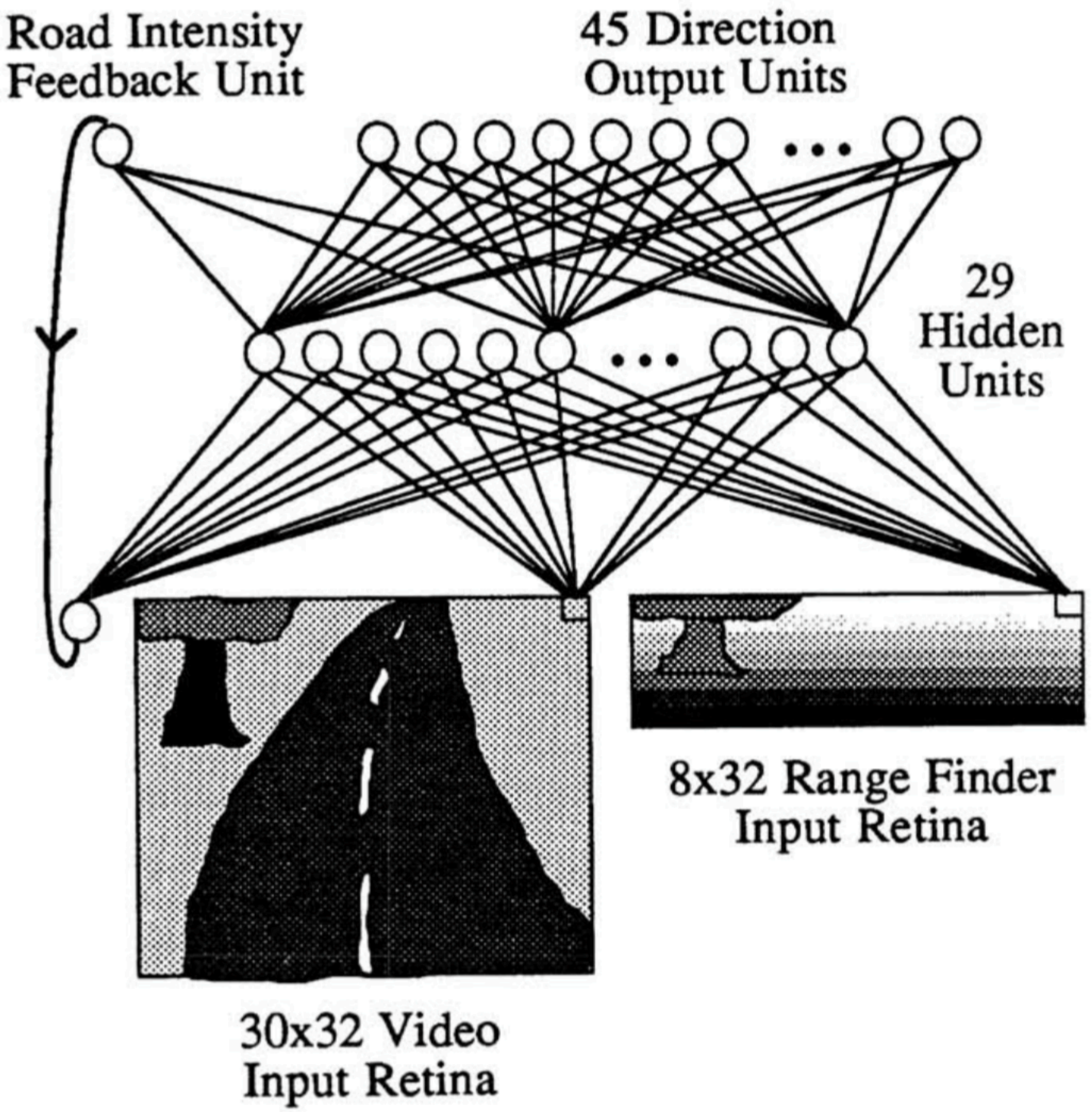


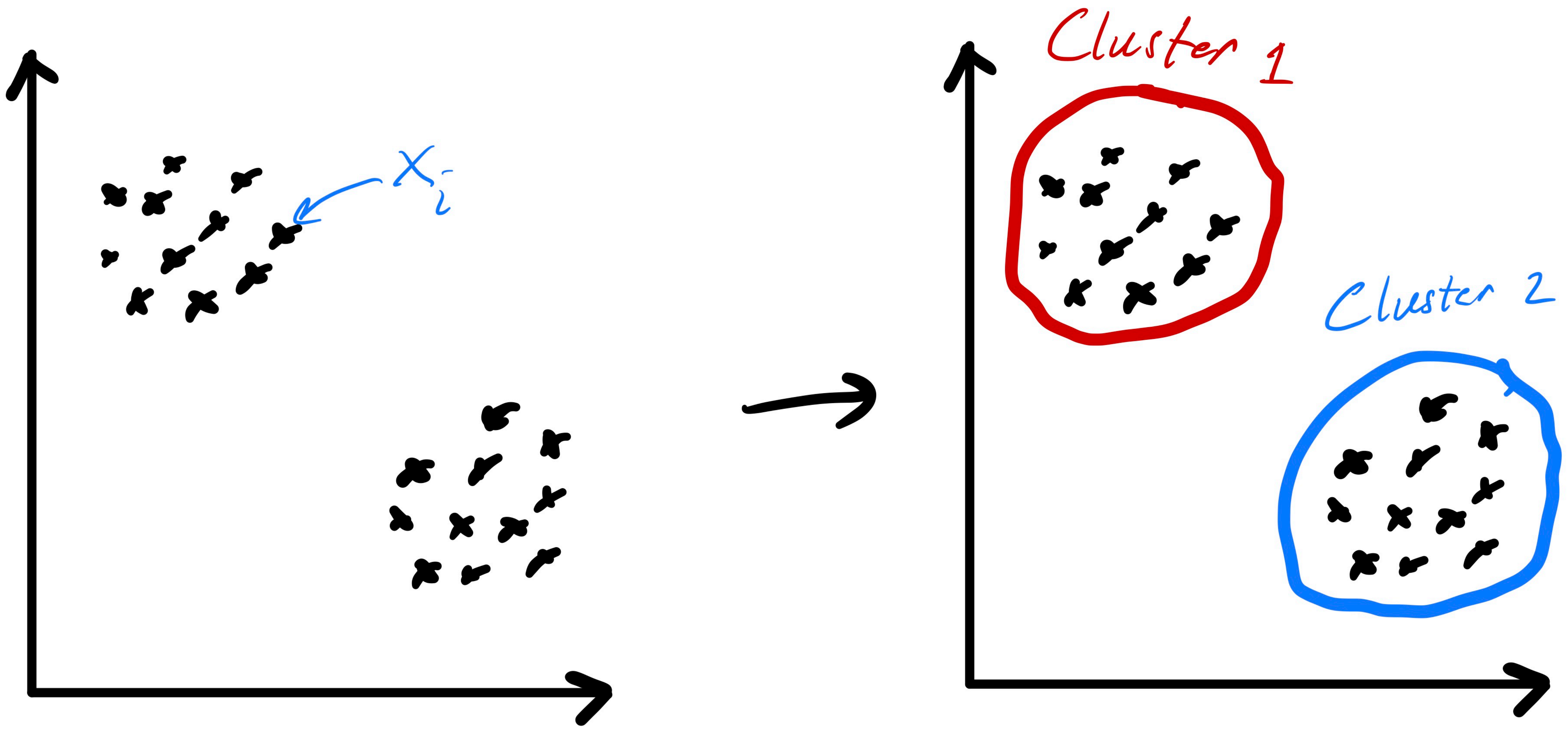
Figure 1: ALVINN Architecture

Unsupervised Learning

Dataset:

$$\mathscr{D} = \{(x_1), \ldots, (x_n)\}, x_i \in \mathbb{R}^d, x_i \sim \mathscr{P}$$

Example: Clustering

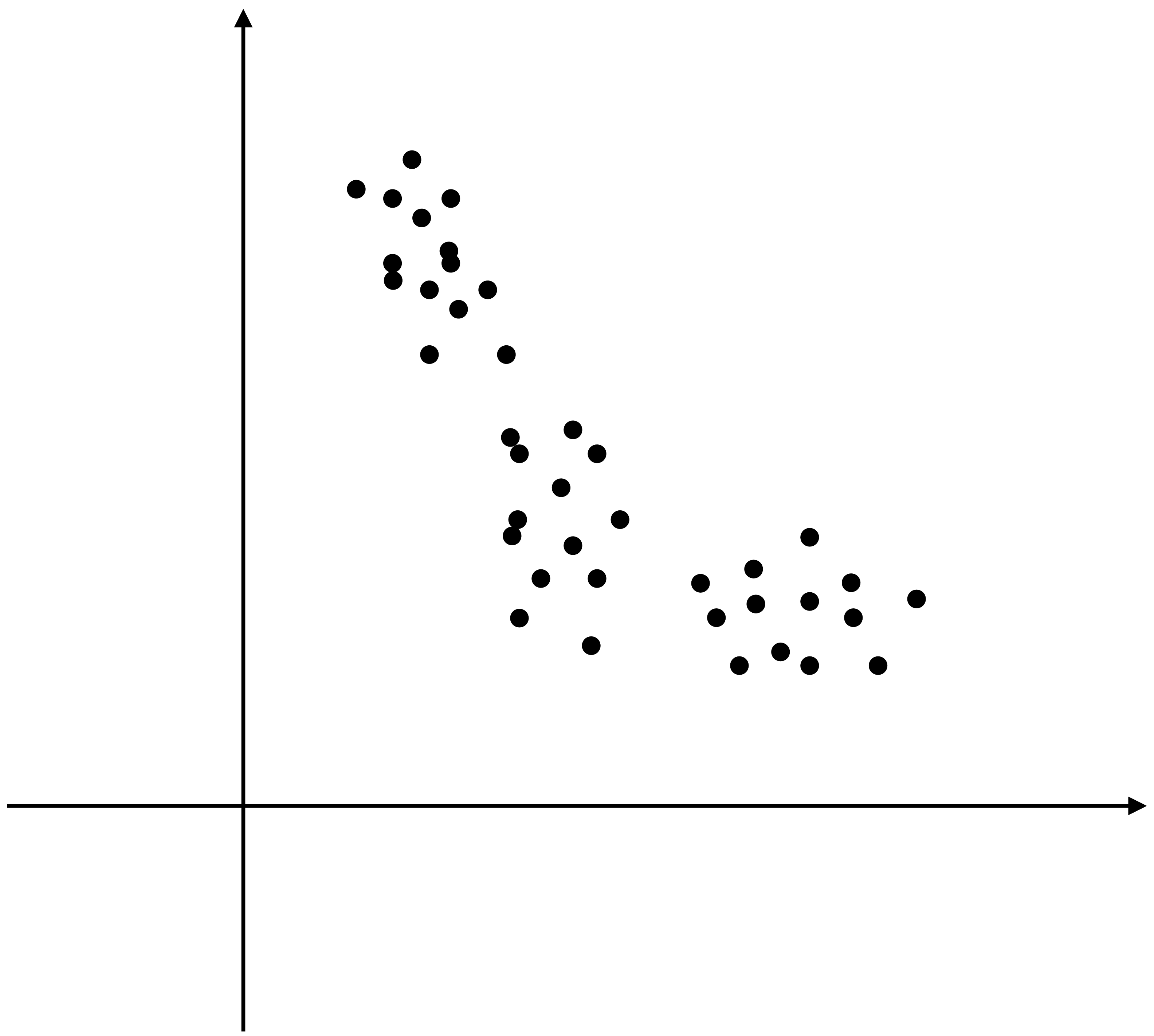


Unsupervised Learning

Dataset:

$$\mathscr{D} = \{(x_1), \ldots, (x_n)\}, x_i \in \mathbb{R}^d, x_i \sim \mathscr{P}$$

Example: distribution estimation



Can we construct a distribution $\hat{\mathscr{P}}$ to approximate $\mathscr{P}$?

Anomaly detection / generative AI

Application of distribution estimation: face generator

Generated images:

Similar images from the dataset

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Generalization

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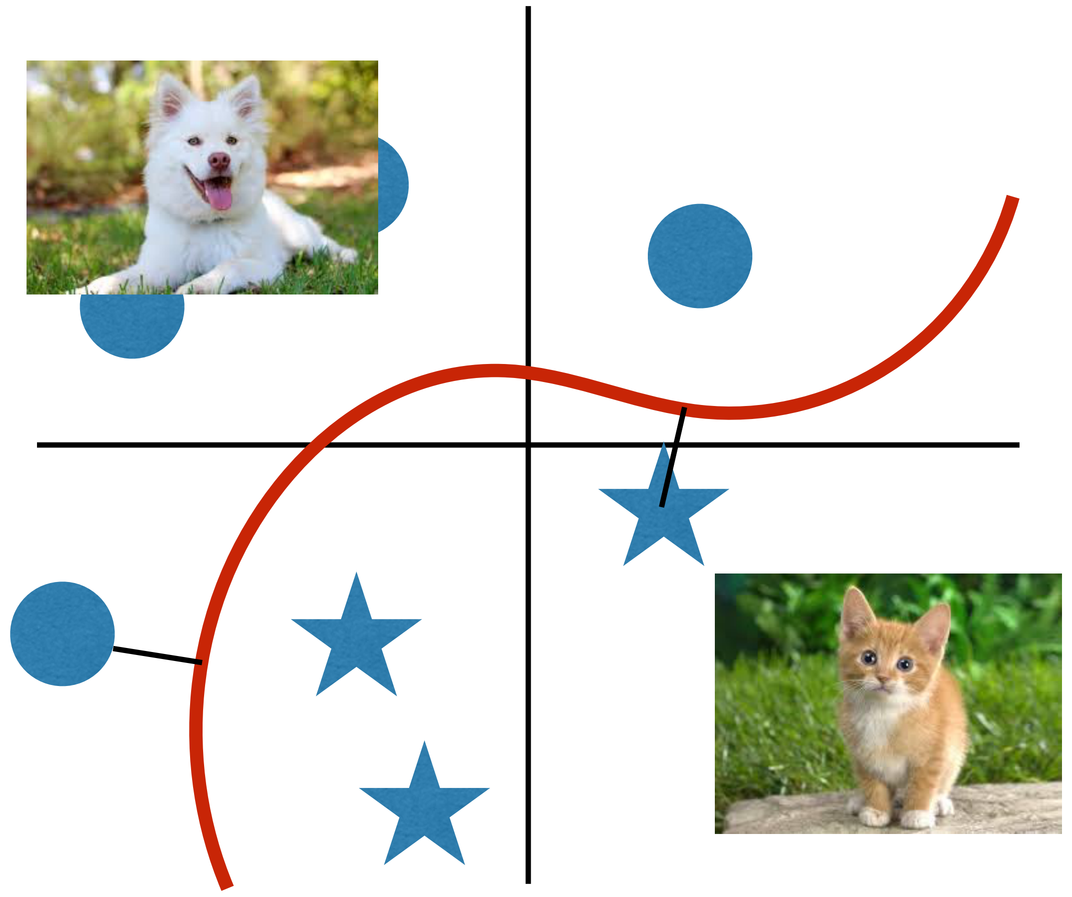
( ,cat) ( ,cat) ( ,dog)

ML model



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

Let's formalize this using distribution

The **Independent and identically distributed** (i.i.d) assumption:

Training data $\mathscr{D}$ is i.i.d sampled from a distribution $\mathscr{P}$, i.e., $x_i, y_i \sim \mathscr{P}, \forall i \in [n]$
(i.e., all pairs are sampled from $\mathscr{P}$, and (x_i, y_i) is independent of others)

We further assume test data is also from $\mathscr{P}$, i.e., $(x, y) \sim \mathscr{P}$

Generalization error: $\mathbb{E}_{x,y\sim\mathscr{P}}\left[\ell(\hat{h}, x, y)\right]$

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

Overfitting

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

Example

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

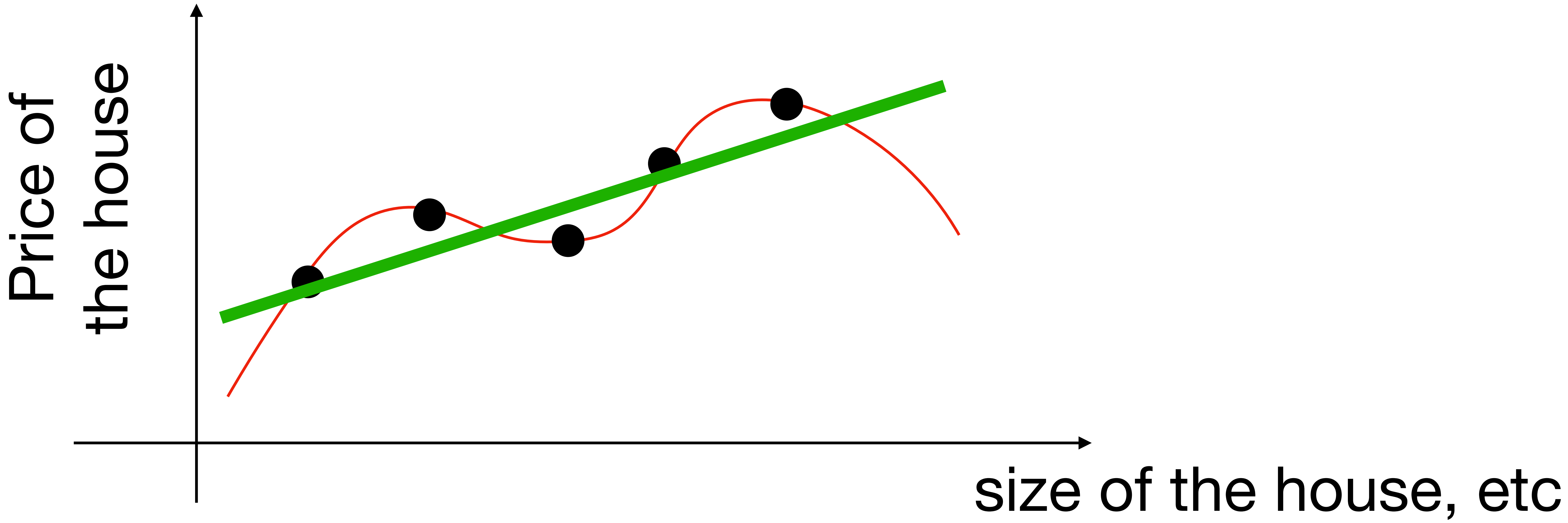
$$\tilde{h}(x) = \begin{cases} y_i & \exists (x_i, y_i) \in \mathcal{D} \text{ w/ } x_i = x \\ -1 & \text{else} \end{cases}$$

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

Overfitting

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

Example



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

Given a training dataset $\mathscr{D}$, we can split it into three sets:

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

$\mathscr{D}_{VA}$: validation set

$\mathscr{D}_{TE}$: test set

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

Selecting models using validation set

We can use validation set to select models, i.e., select hypothesis class, tune parameters, etc

Small avg error on $\mathscr{D}_{TR}$ but larger avg error on $\mathscr{D}_{VA}$ indicates overfitting

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

Do not use test set to train/select models

We should not touch test set during training!

This makes sure that the test set $\mathscr{D}_{TE}$ is independent of our model $\hat{h}$

Such independence implies that:

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

(Due to law of large numbers)

Other ways to split the data?

Can we split data based on features, or labels?

Summary

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 $\mathscr{D}_{VA}$