Machine Learning Basics

Wen Sun

Cornell University Artificial Intelligence (CUAI)

👍 CUAI is a unique club at Cornell that promotes undergraduate-led ML research

👍 We've published 4 NeurIPS, 1 ICML, 1 ICLR, and 1 ICCV paper since 2018

Our Mission

- ❑ Prepare our members to tackle cutting-edge research topics
- ❑ Connect undergraduates with Cornell faculty to explore shared interests
- ❑ Provide research credit and financial support for compute resources and conference travel

We are recruiting! 👉

Announcement:

Outline for Today:

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

2. Generalization

3. Training / validation / testing

Classification

Dataset $\mathscr{D}$

$\Big($  ,cat $\Big)$ $\Big($  ,cat $\Big)$ $\Big($  ,dog $\Big)$

Classification

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ML model

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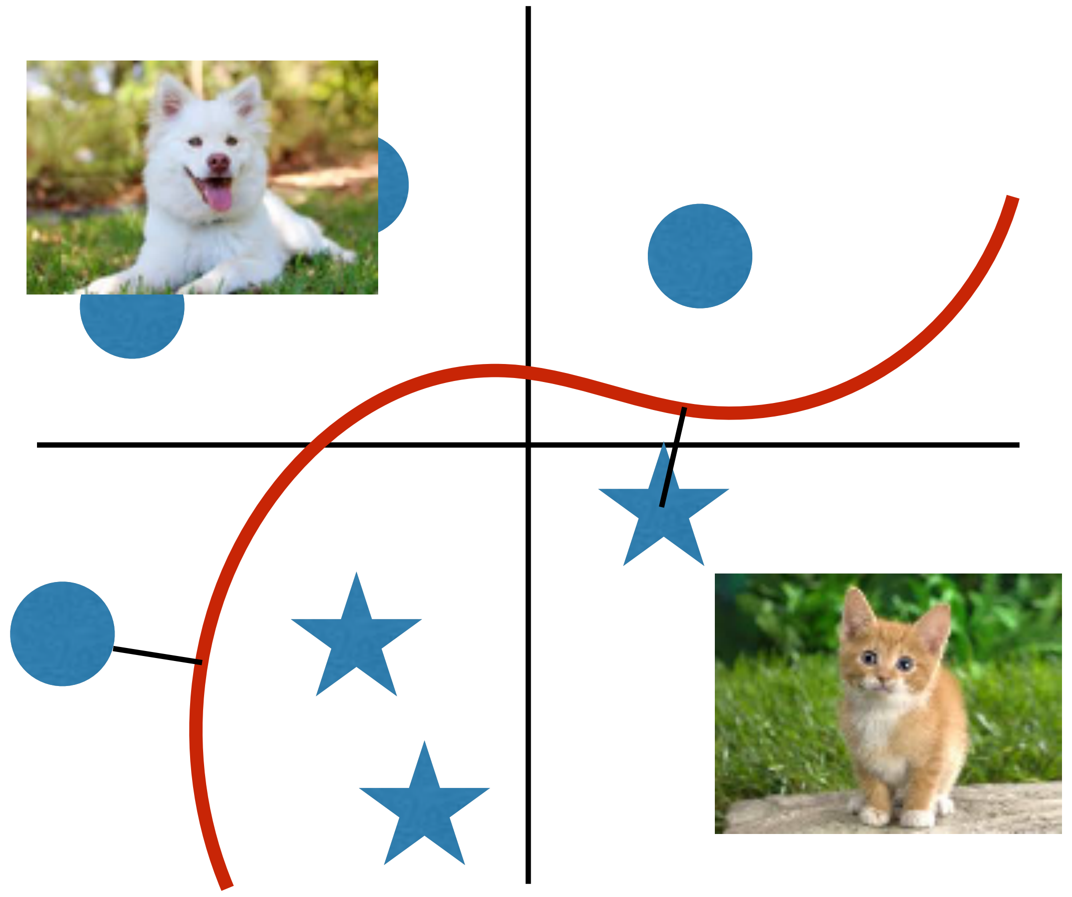

Mathematical formulation of the pipeline

Dataset:

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

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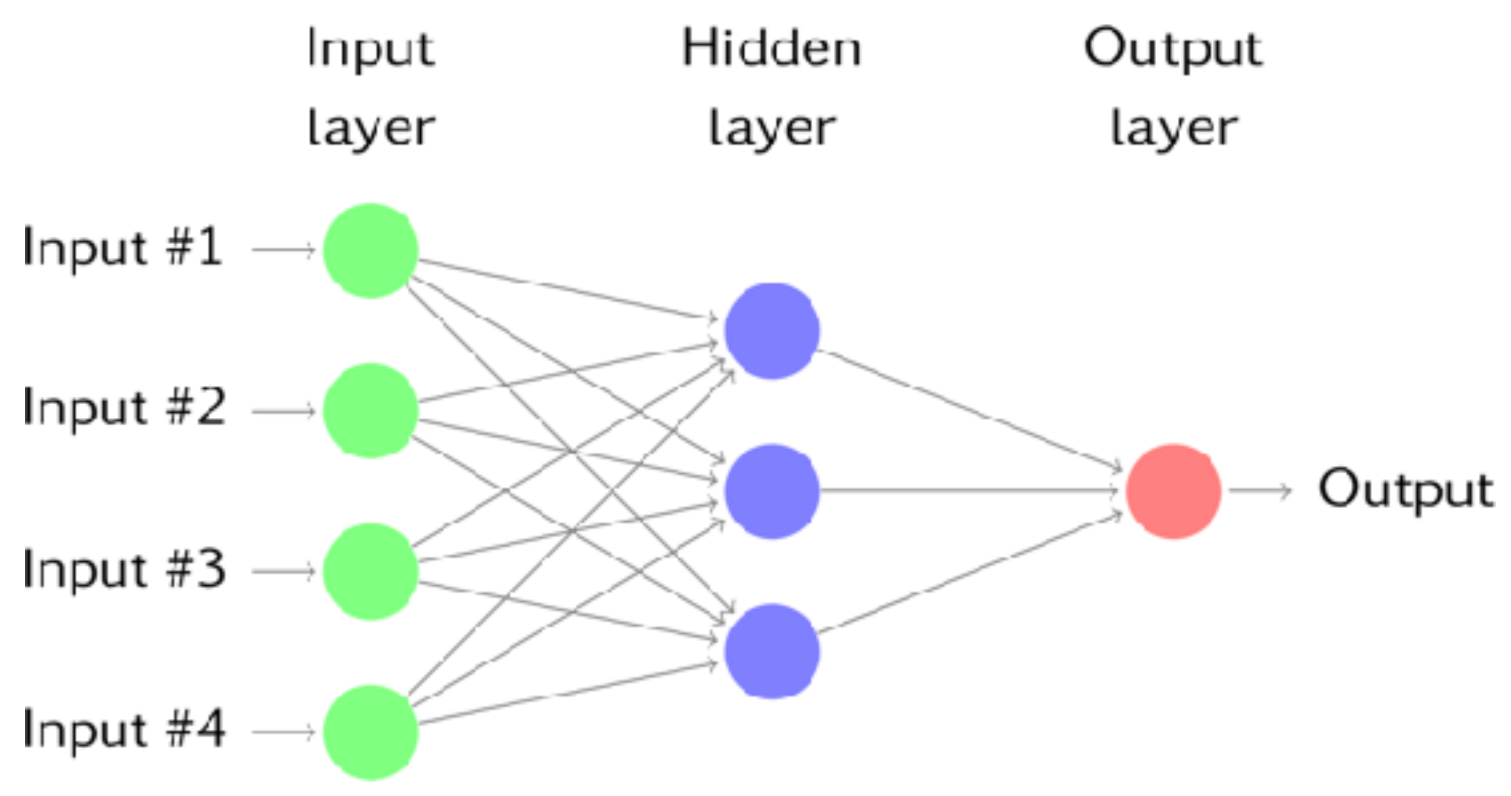

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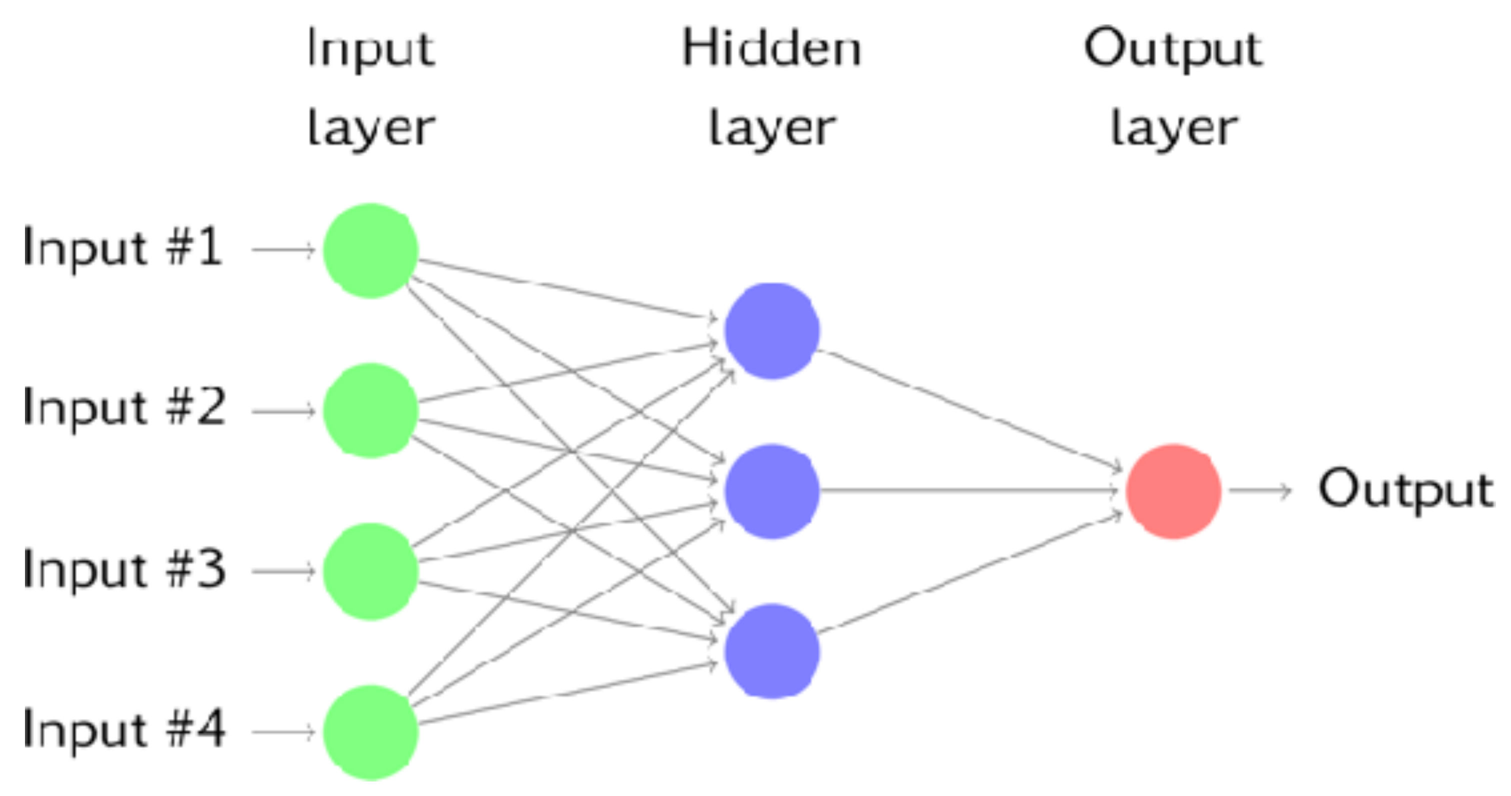

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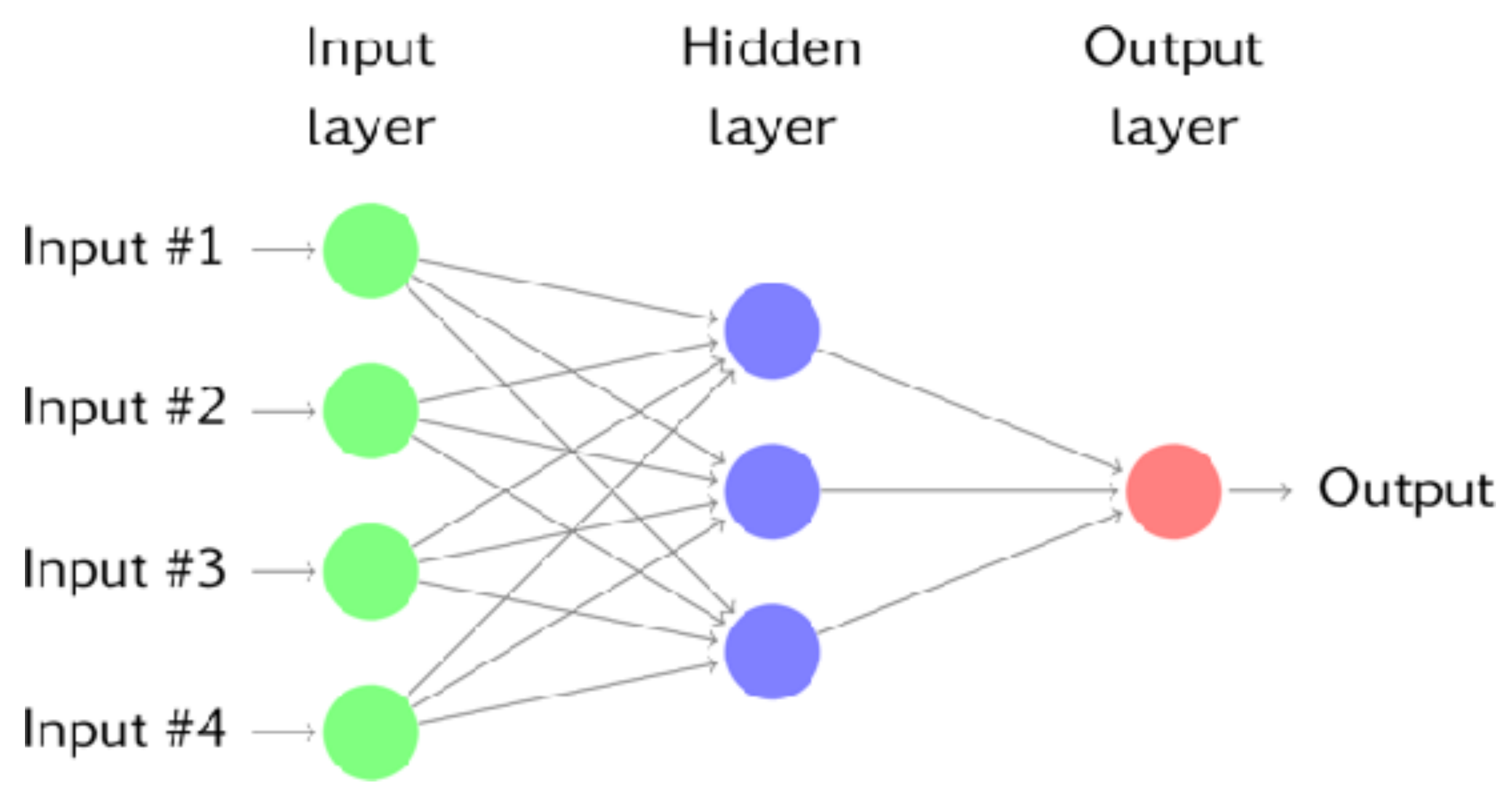

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Hypothesis class

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

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

Examples of hypothesis

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

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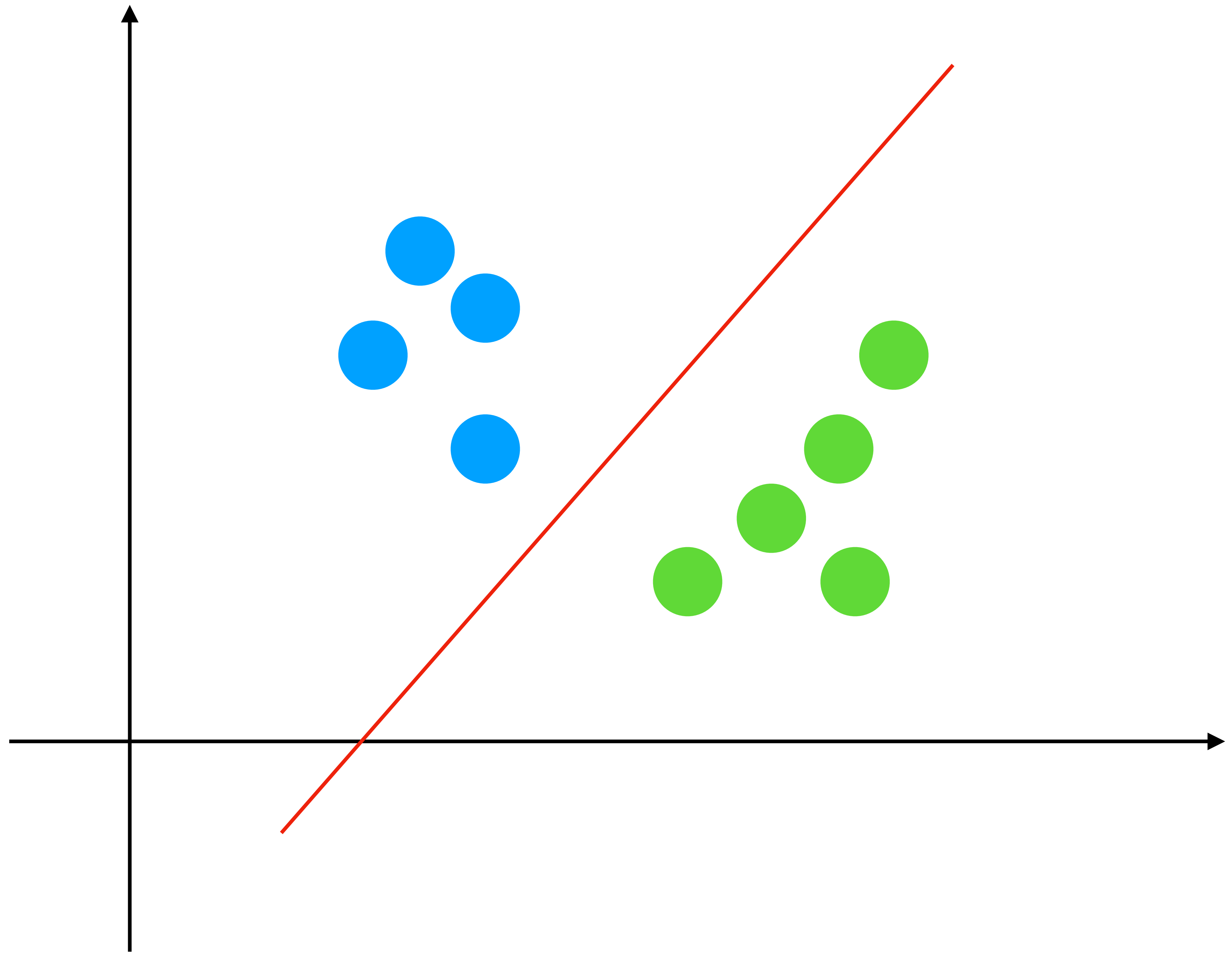
$\mathscr{H}$ contains all possible linear functions



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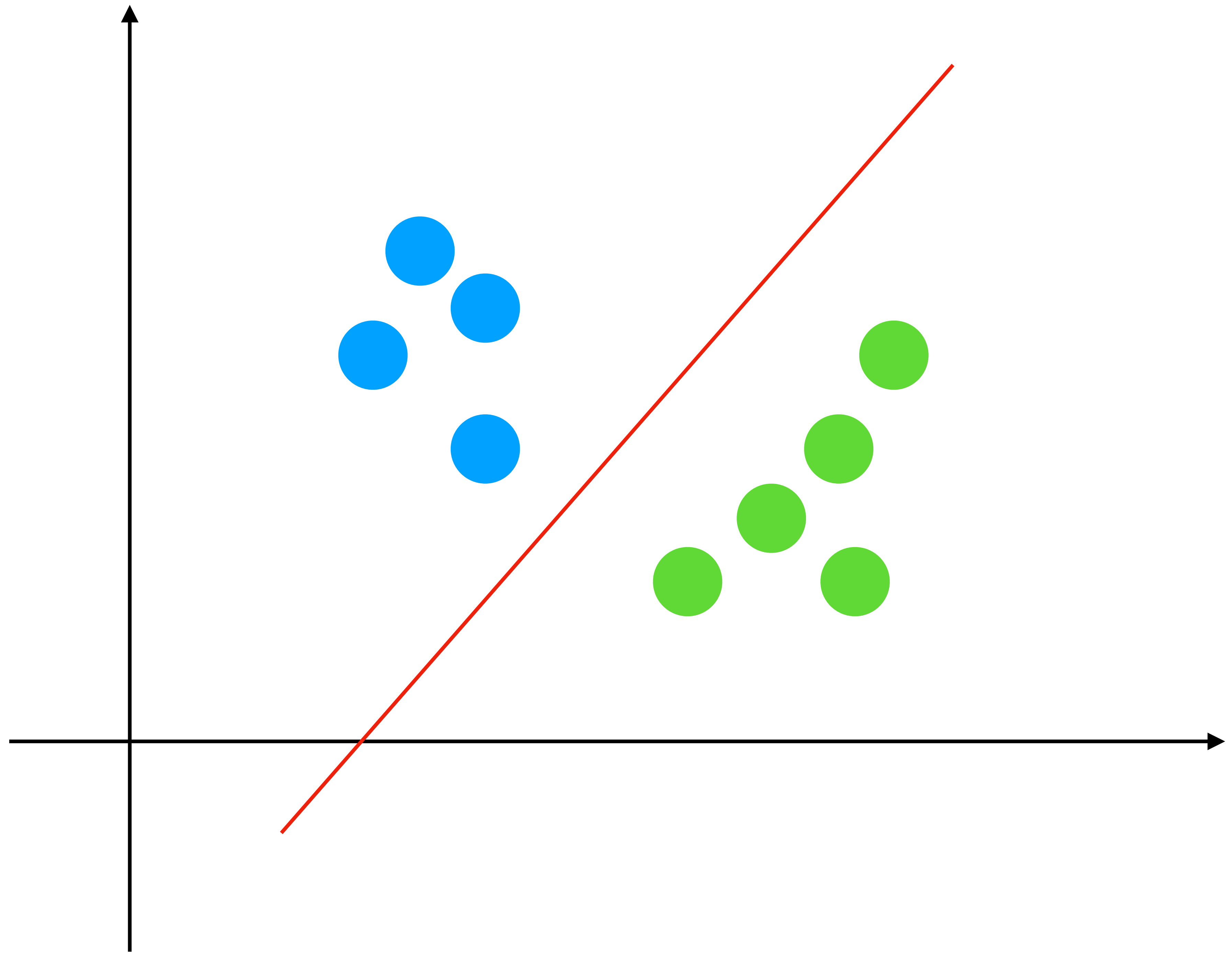
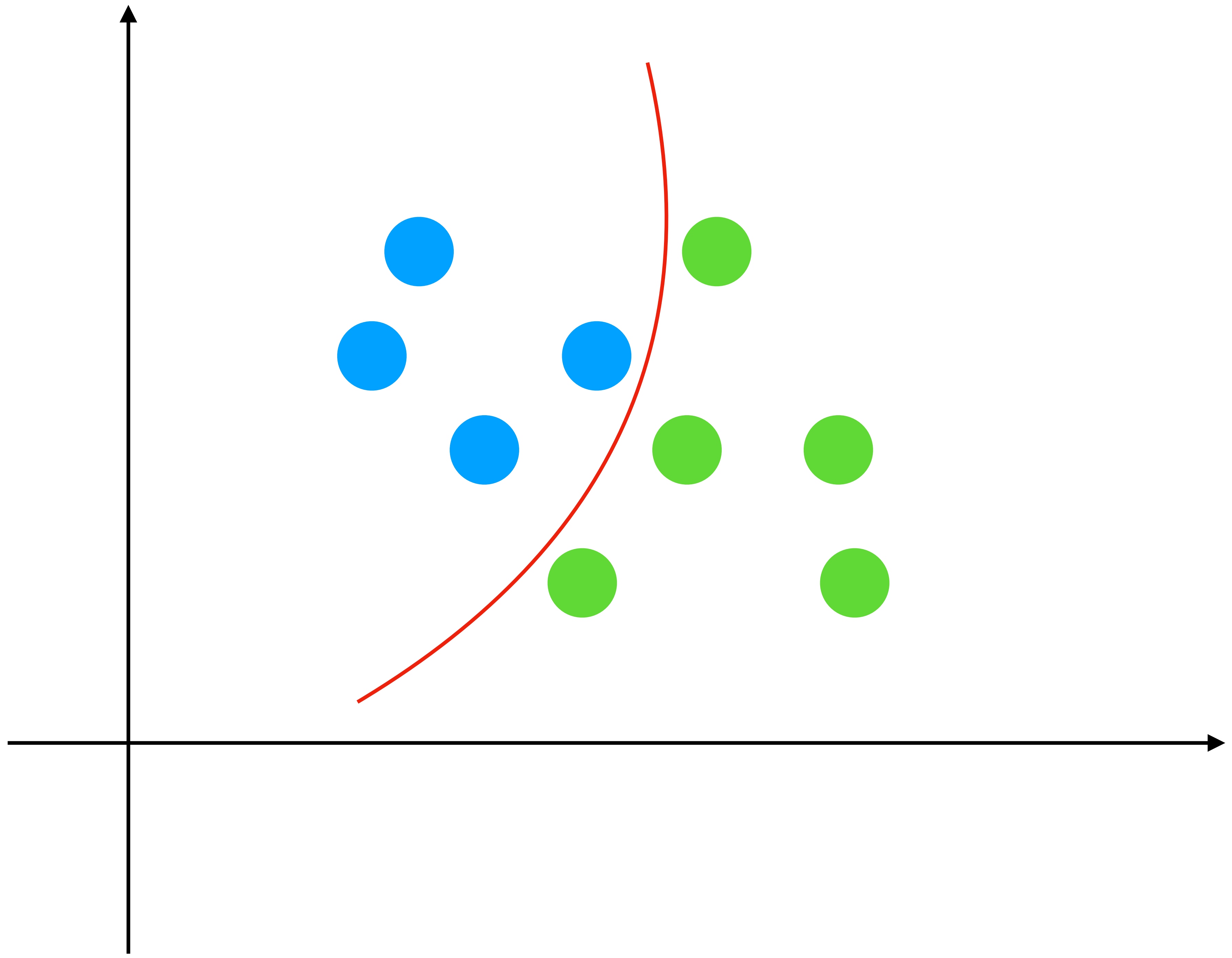


Ex: h is nonlinear $h(x) = \text{sign}(w^\top(\text{relu}(Ax)))$;
$\mathcal{H}$ contains all possible one-layer NN



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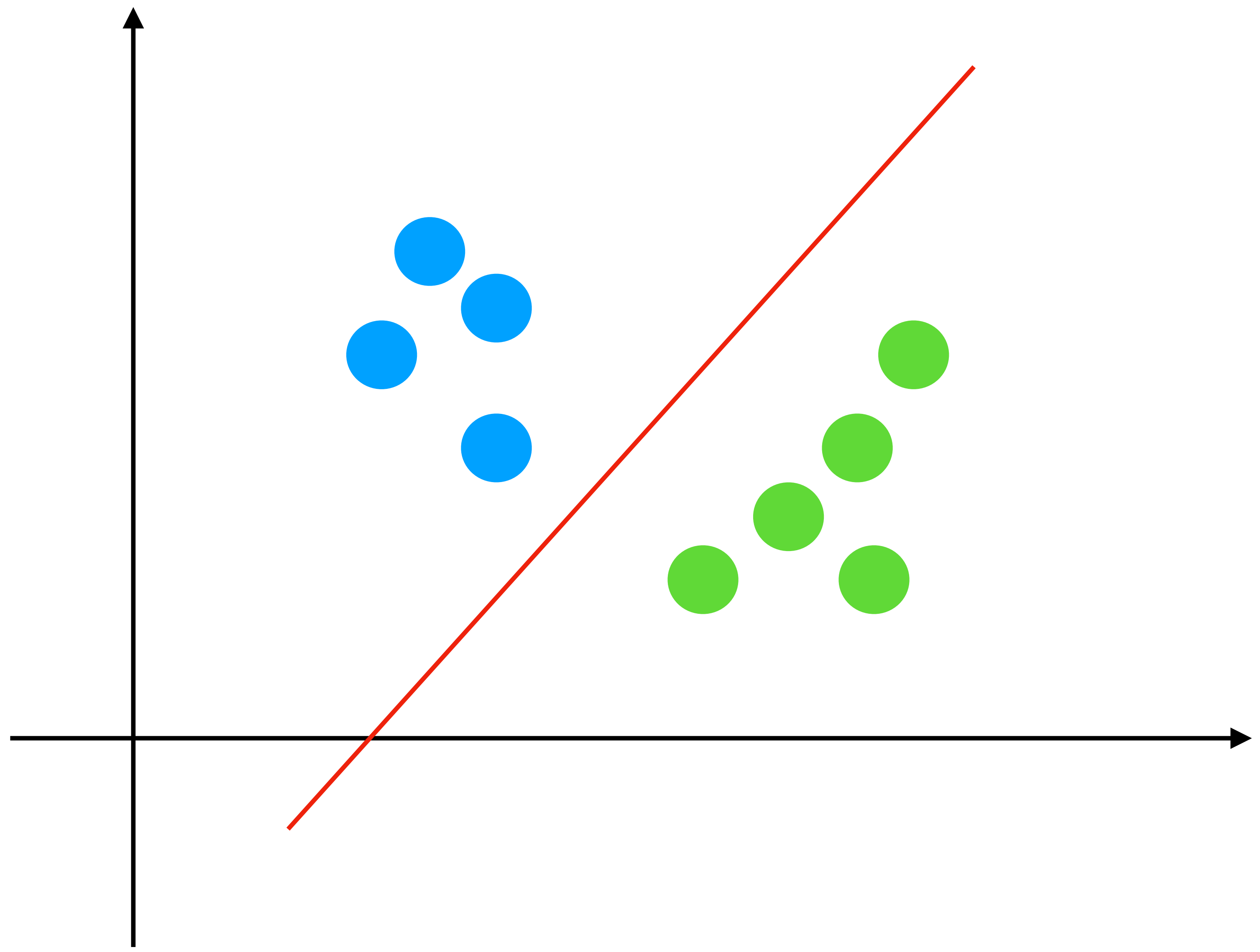

We use prior knowledge (i.e., we believe linear function is enough) to design an ML algorithm here

The Loss Function

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Examples:

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

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

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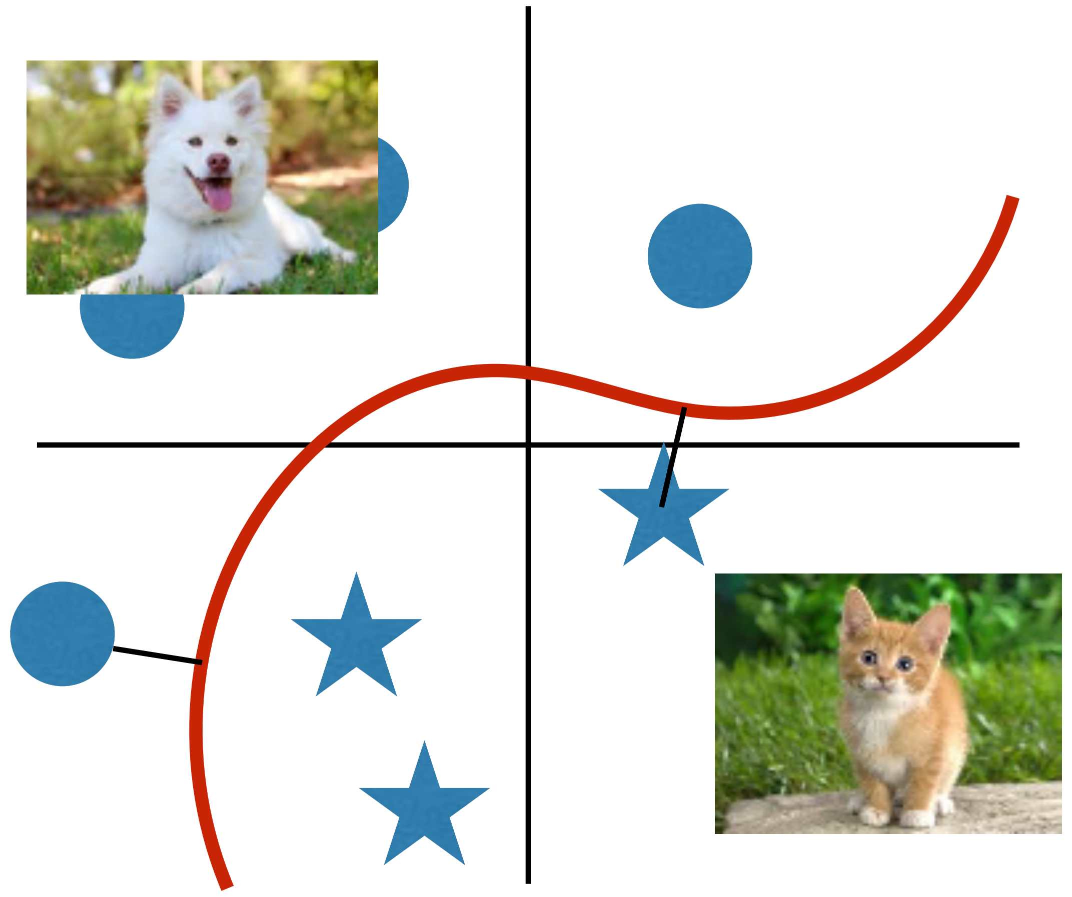

Regression

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Training: minimizing mean squared error (MSE)

$$\arg\min_\theta \sum_i (\theta^\top x_i - y_i)^2 / n$$

An Autonomous Land Vehicle In A Neural Network *[Pomerleau, NIPS '88]*

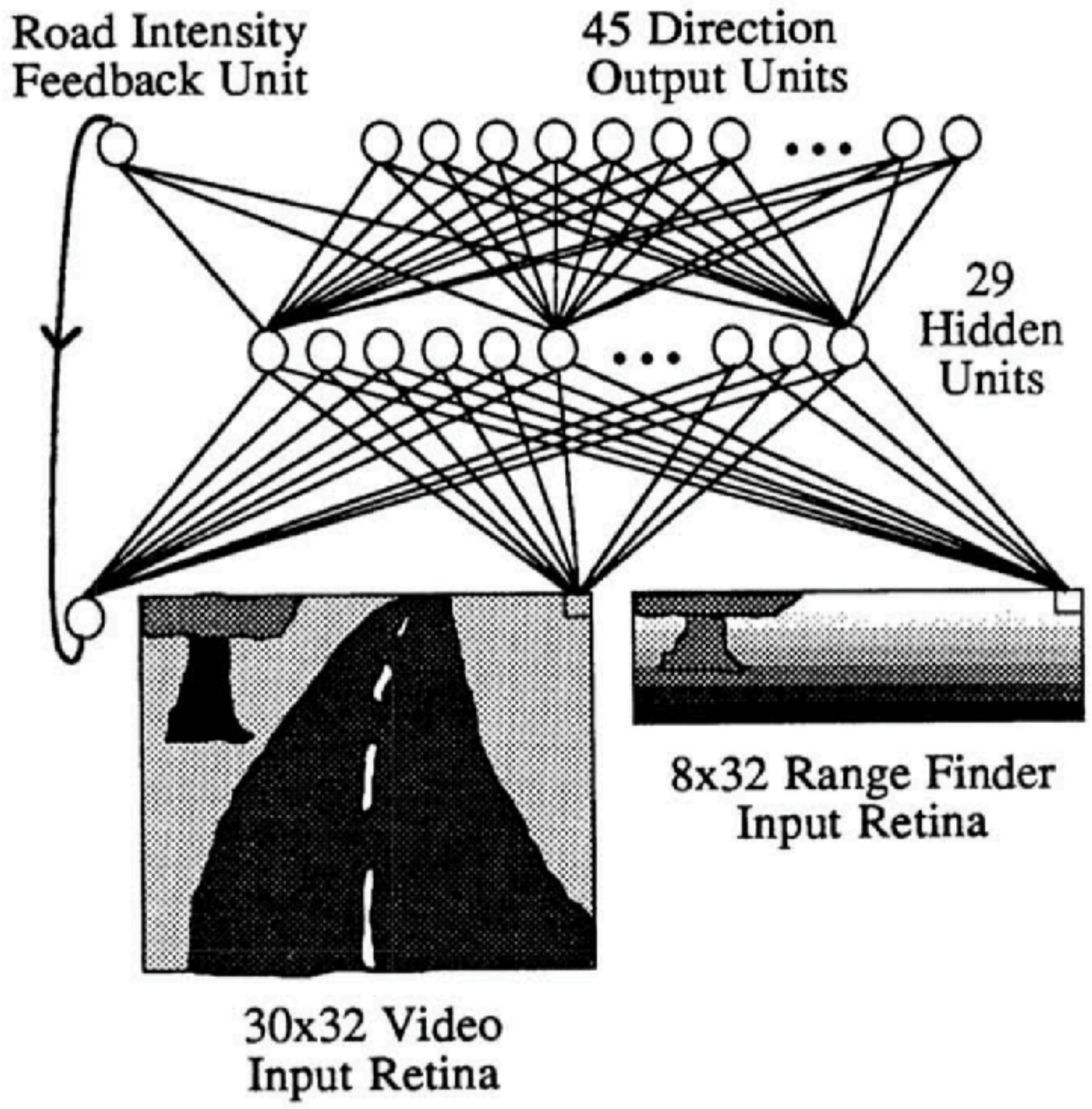

Figure 1: ALVINN Architecture

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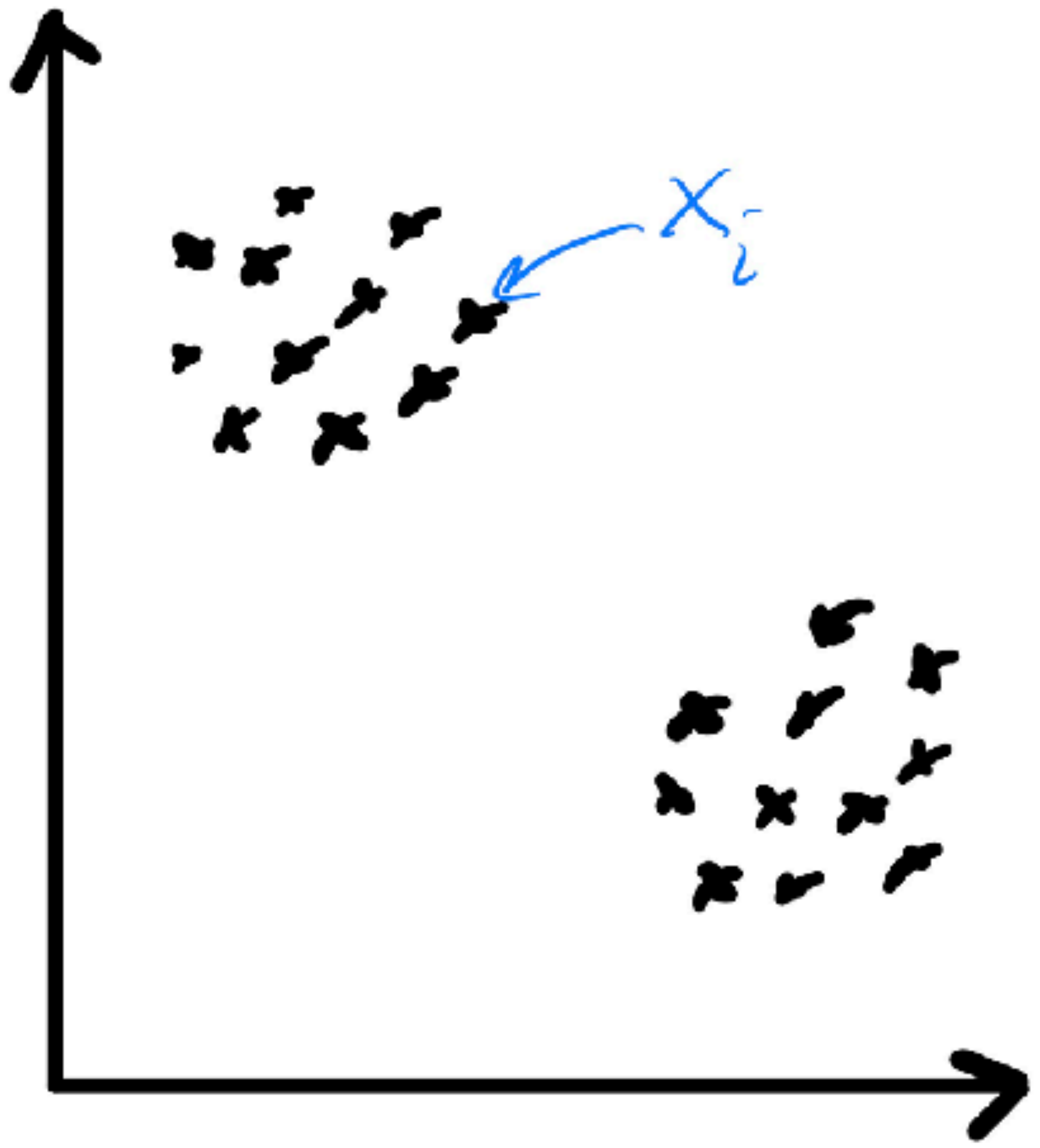

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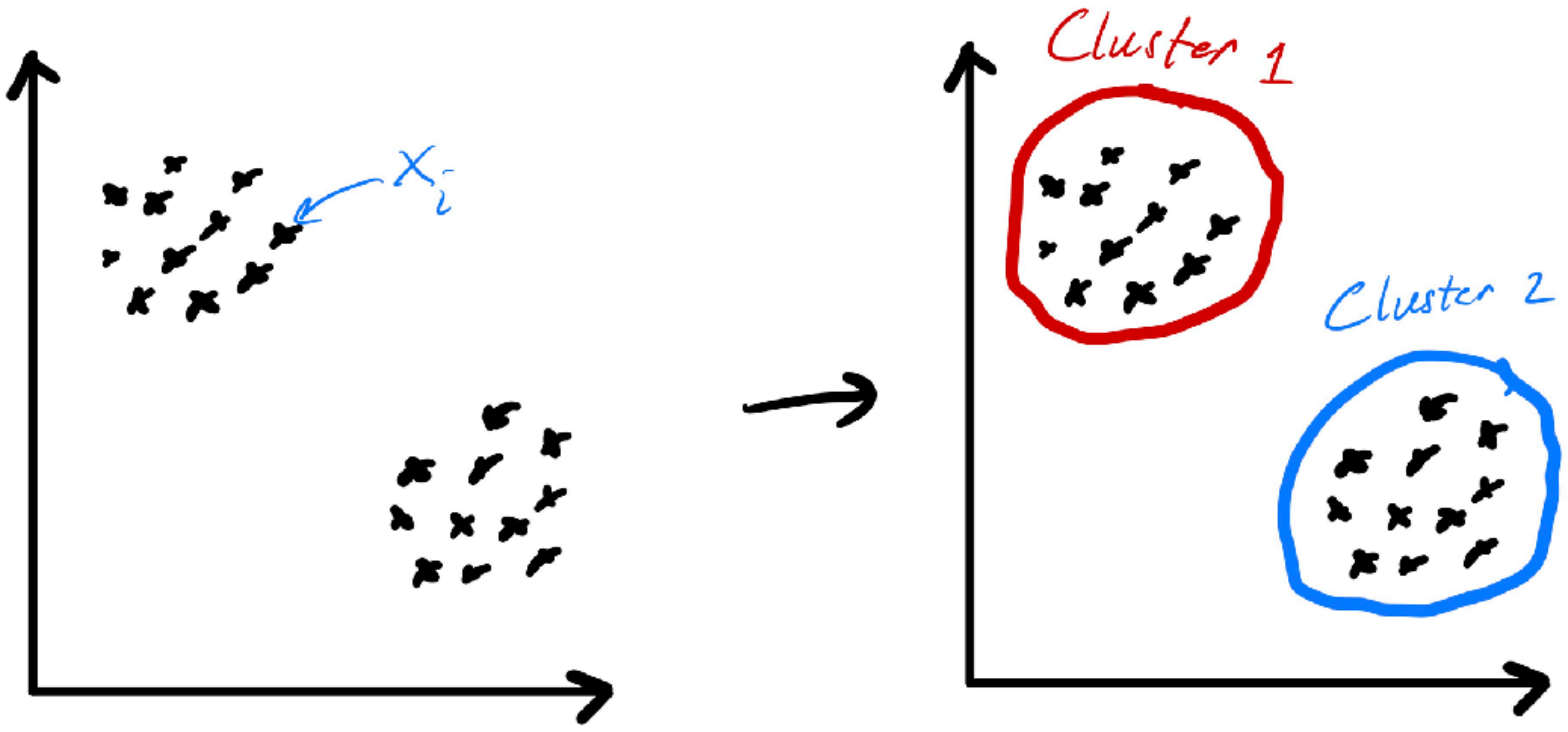

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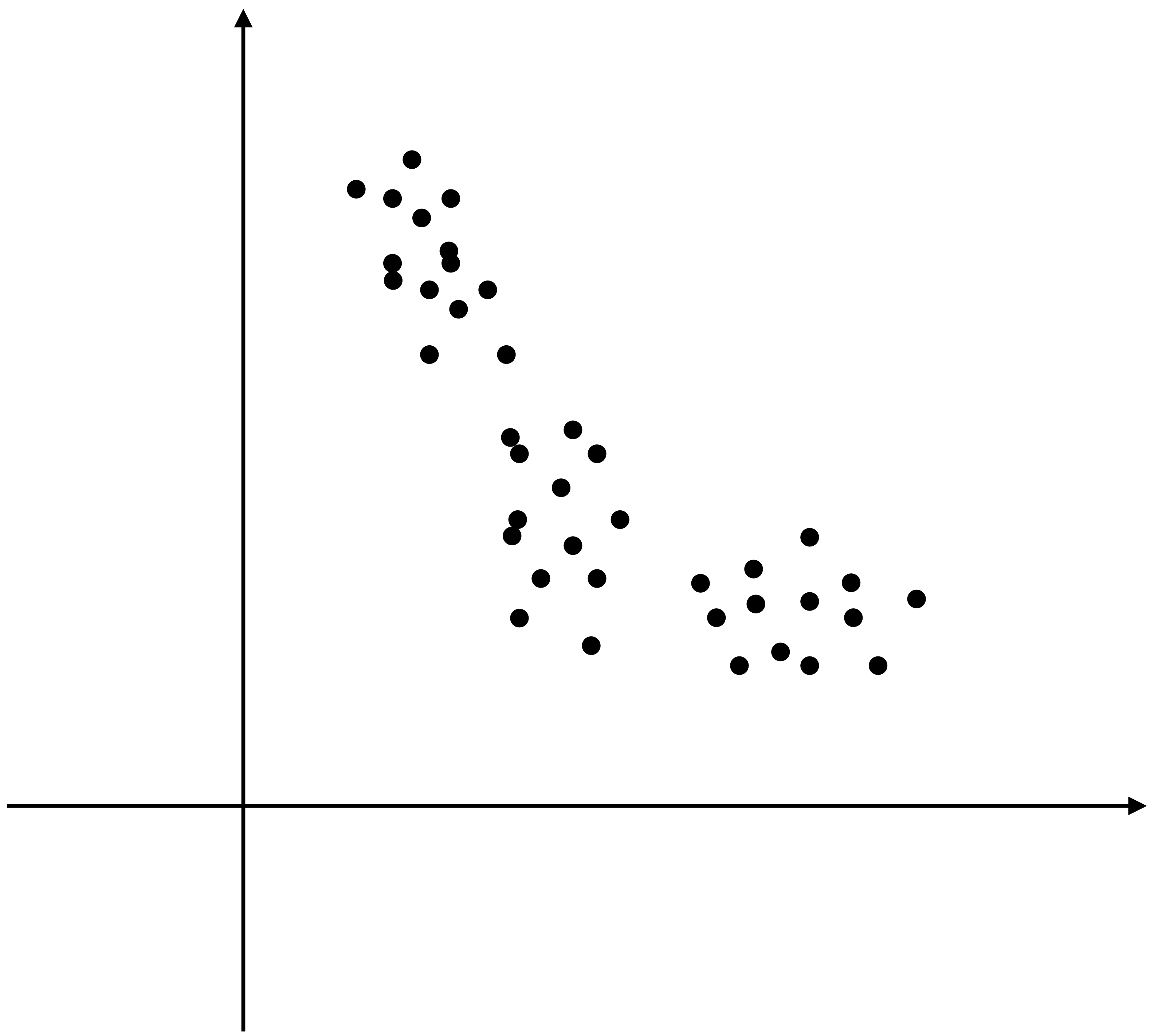
Example: Density estimation / Anomaly detection



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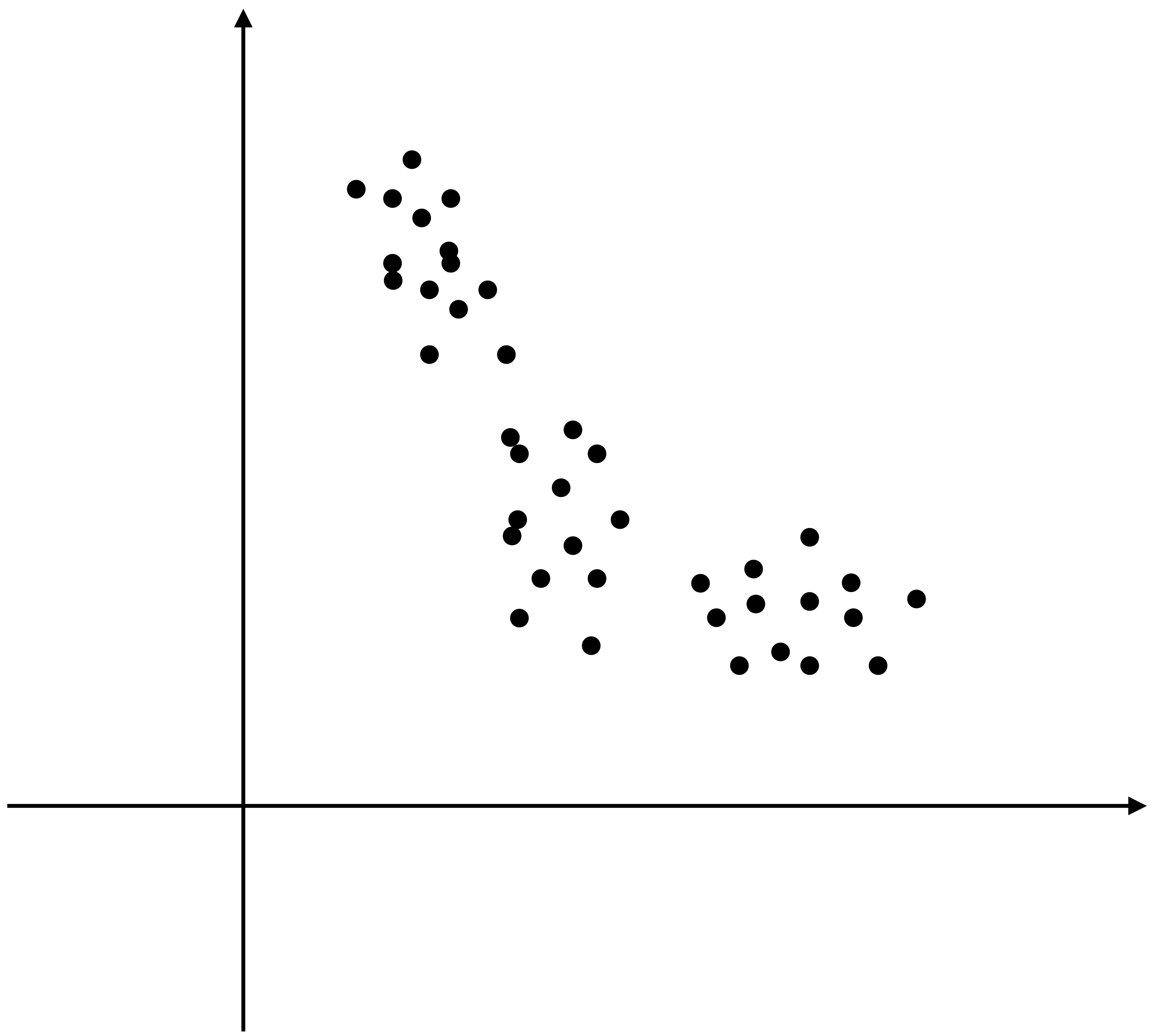

Can we construct a distribution $\hat{\mathscr{P}}$ to approximate $\mathscr{P}$?

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Generalization

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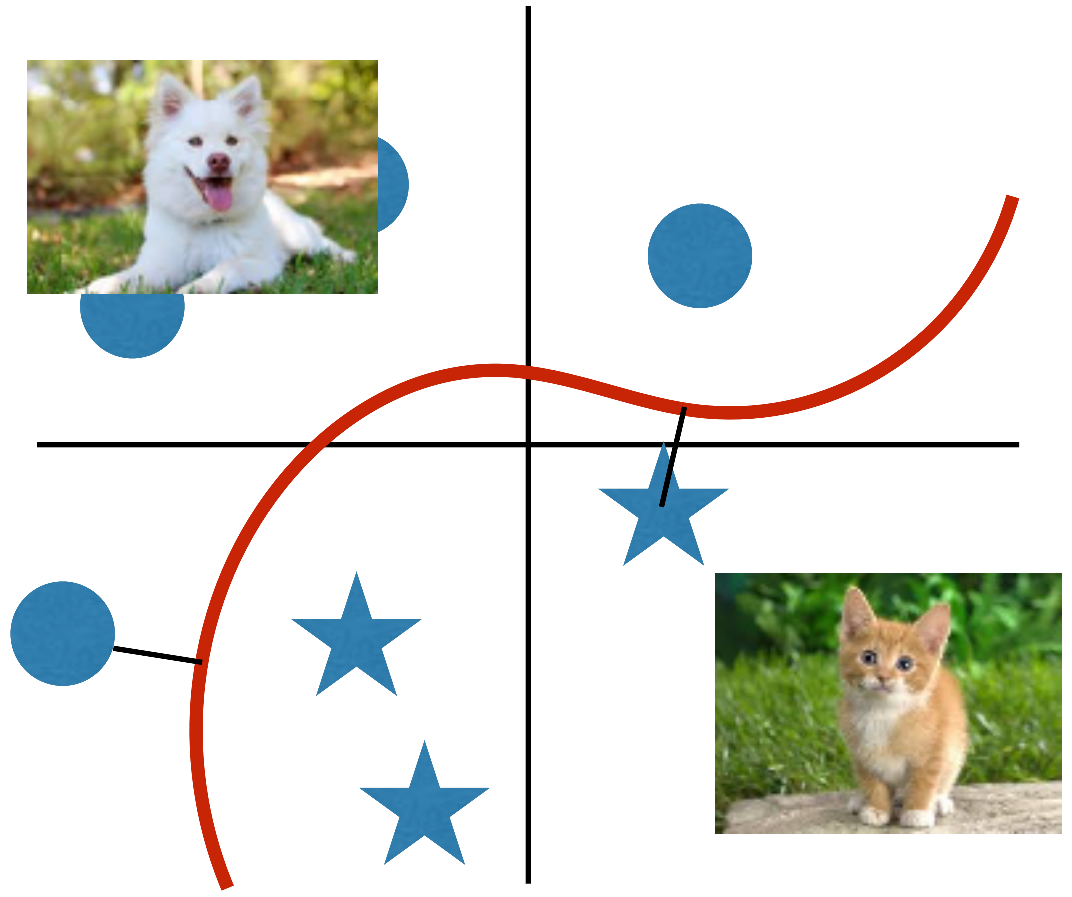
ML model



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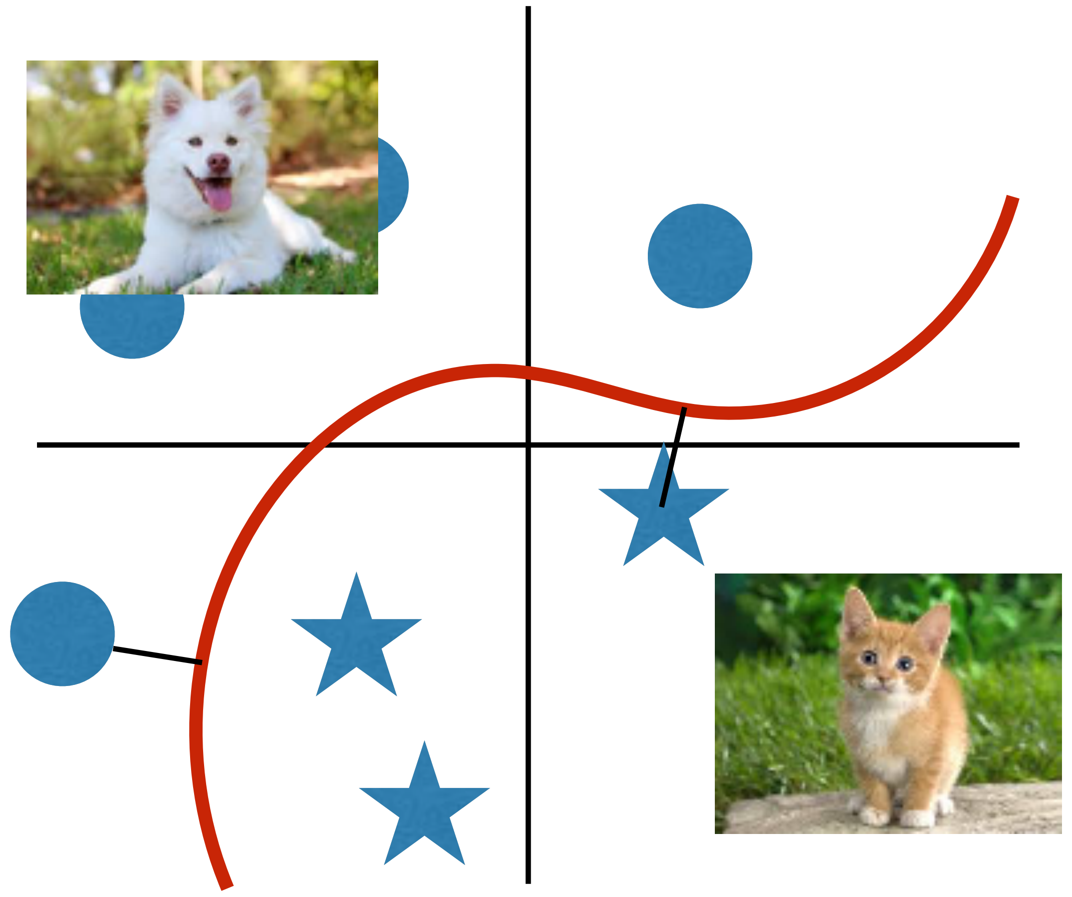

Generalization: how well can our trained model do on <u>unseen test examples</u>?

Let’s formalize this using distribution

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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

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Example

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

$$\tilde{h}(x) = \begin{cases} y_i & \exists (x_i, y_i) \in \mathscr{D} \text{ w/ } x_i = x \\ 0 & \text{else} \end{cases}$$

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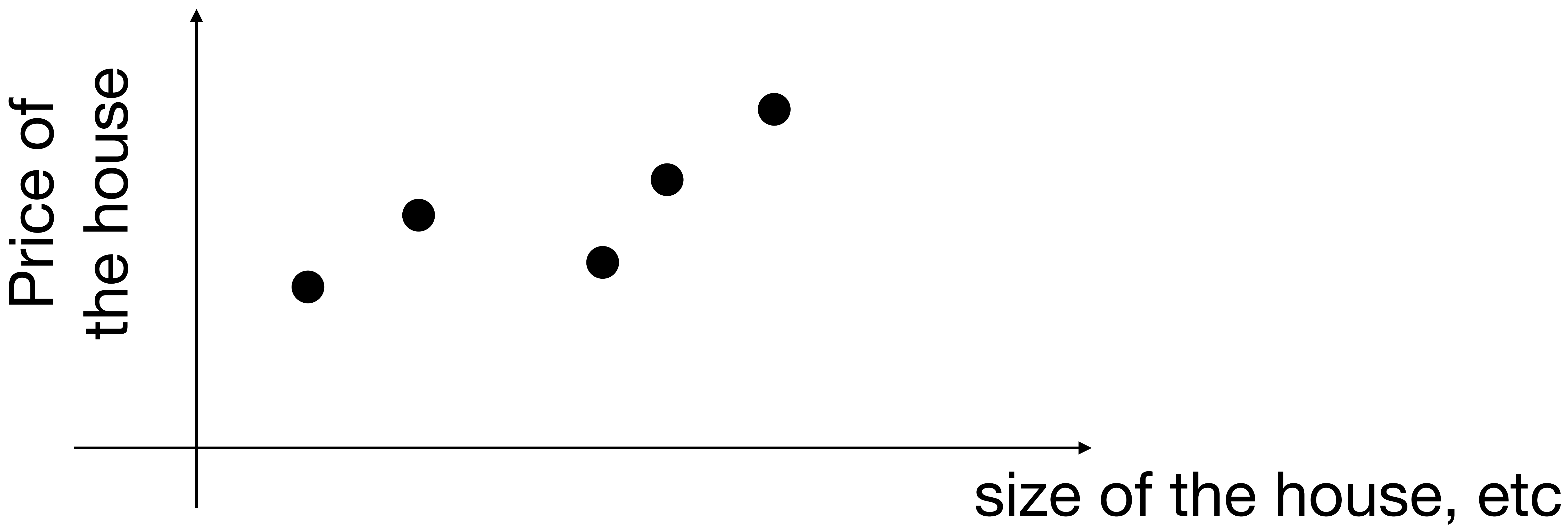

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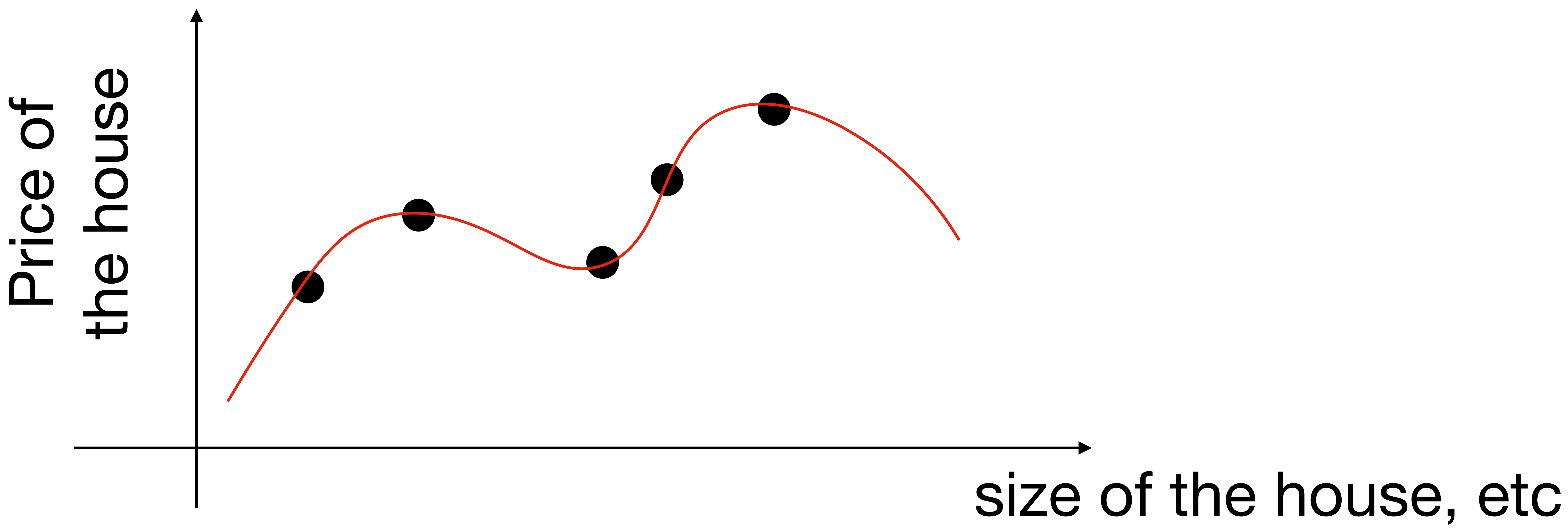

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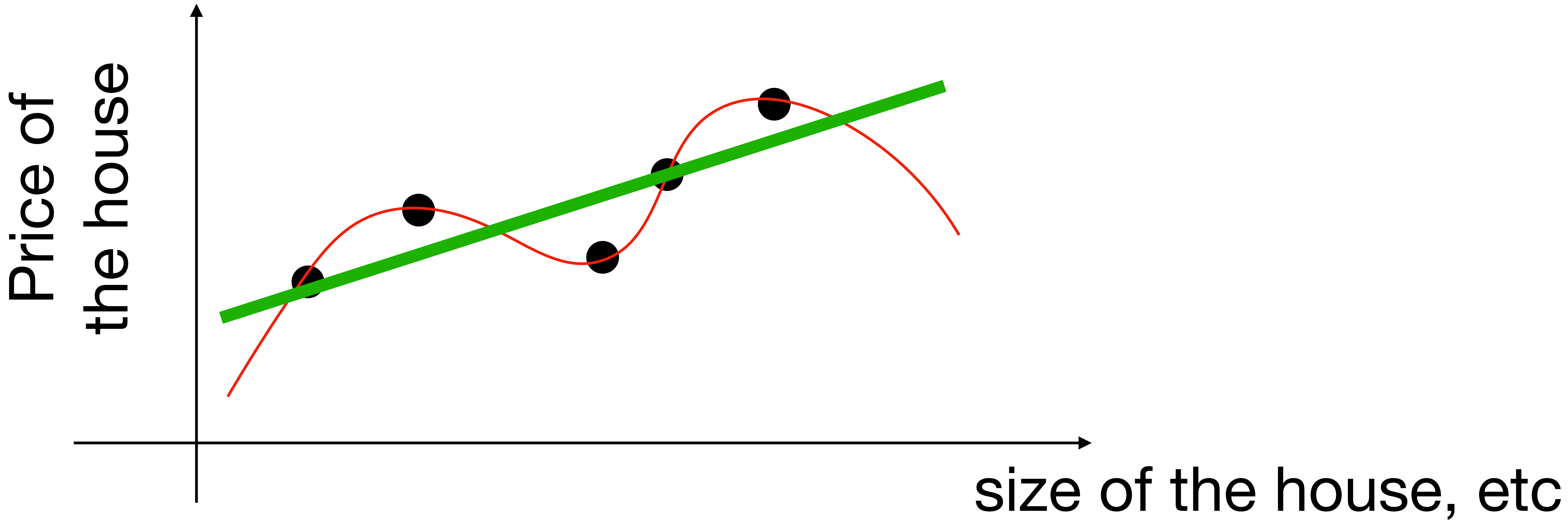

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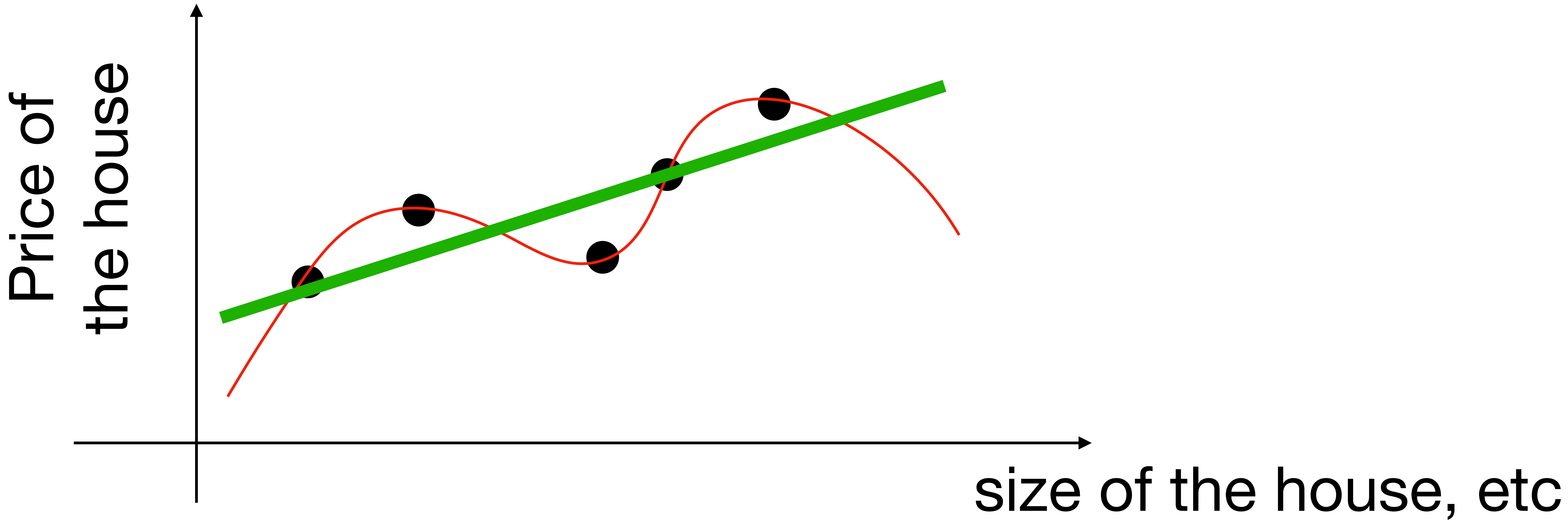

Training error = 0 (e.g., we probably overfit to noises), but could do terribly on test examples

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

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

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

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

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⬇

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Such independence implies that:

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

(Due to law of large numbers)

Select / train models on small dataset

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- Train model $\hat{h}$ on D_{TR}
- Validate on the i'th fold (i.e., $\mathscr{D}_{VR}$ = i'th fold)

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- Validate on the i'th fold (i.e., $\mathscr{D}_{VR}$ = i'th fold)

Average K validation errors

Select / train models on small dataset

What if our original dataset is quite small, e.g., $n = 100$
(very possible in medical applications!)

K-fold cross validation

Split the data into K folds (e.g., K = 10 or 20)

For $i = 1 \rightarrow K$:

- $\mathscr{D}_{TR}$: all others folds except the i'th fold
- Train model $\hat{h}$ on D_{TR}
- Validate on the i'th fold (i.e., $\mathscr{D}_{VR}$ = i'th fold)

Average K validation errors

When K = n, this is leave-one-out cross validation

Summary

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