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Introduction to Machine Learning

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Types of learning

Learning with a teacher

The concept of **feedback** from a teacher is central in ML:

1. the model makes a prediction,
2. a teacher compares the model prediction with its prediction and gives back a feedback of how right is the prediction,
3. the model uses this feedback to improve its prediction.

Supervised learning

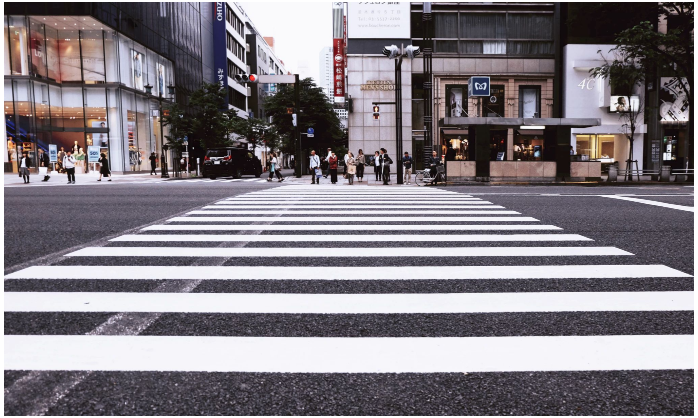
The teacher (e.g., annotators) provides targets for some examples.

- **Regression**: the targets are real-valued variables.
- **Classification**: the targets are categorical variables.
    - **Multi-class**: choose only one class among a predefined set.
    - **Multi-label**: choose all relevant classes among a predefined set.

$$z = (x, y)$$

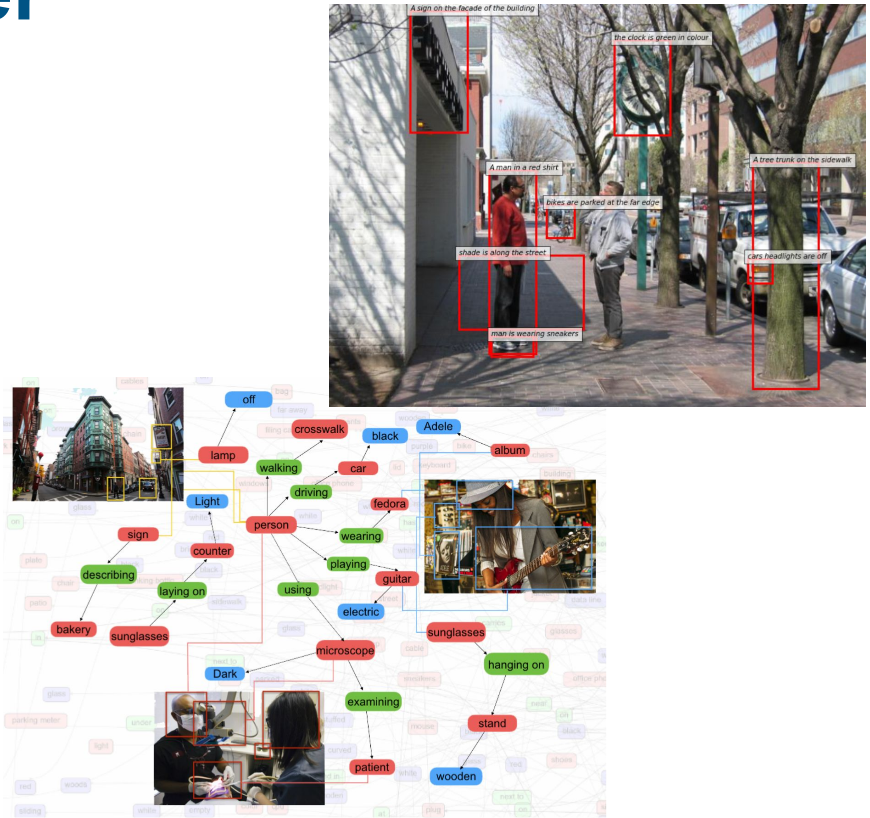
Helpfulness of the teacher

Different levels of information



Source: Daryan Shamkhali, Unsplash

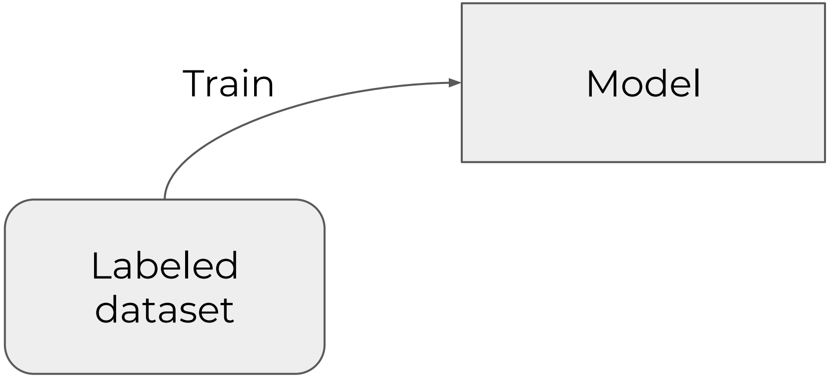
Labels: car, person, tree



Source: Visual Genome dataset

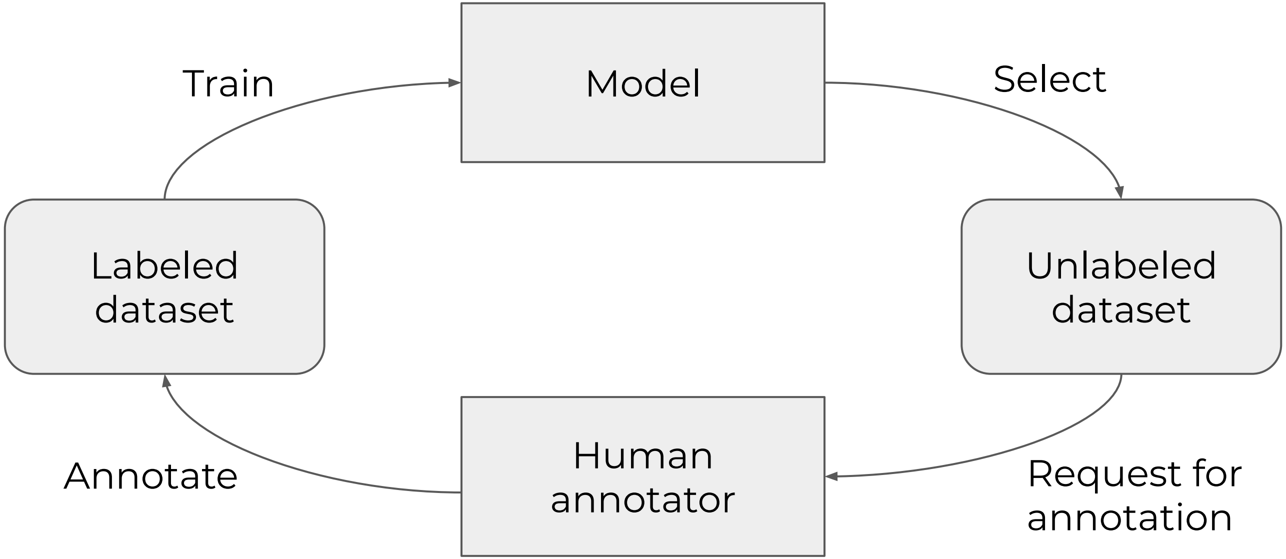
Active vs. passive learning

Passive learning: the learning algorithm has access only to a static dataset provided by the teacher.



Active vs. passive learning

Active learning: the learning algorithm can interact with the teacher to annotate new examples.

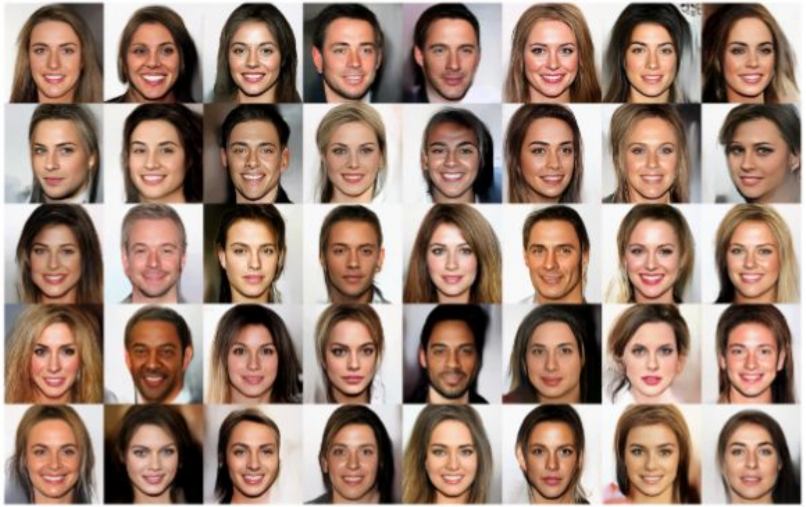


Unsupervised learning

- We only have the high-dimensional data (text, images, videos, etc.)
- Very weak signal from the teacher generated by the choice of a task:
    - Predict next words,
    - Reconstruction - denoising,
    - Predict if the video is playing in reverse,
- Probabilistic approaches in high-dimensional space.

Unsupervised learning: applications

- Clustering
- Anomaly detection
- **Data generation**:
  - **Image**, speech, text synthesis,
  - model-based control, ...
- Semi-supervised learning.



Source: Kingma, Durk P., and Prafulla Dhariwal. "Glow: Generative flow with invertible 1x1 convolutions." In Advances in Neural Information Processing Systems, pp. 10215-10224. 2018.

Online vs. batch learning protocol

- **Online learning**: each example must be treated on-the-fly and then discarded. (Hard)
- **Batch learning**: the examples are gathered in a batch and processed together multiple times. (used in deep learning)
- Most of the talks will concern **supervised statistical batch learning with a passive learning algorithm**.

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Supervised learning

Statistical learning framework

- Domain set $\mathcal{X}$: set of objects we want to annotate.
- Label set $\mathcal{Y}$: set of possible labels.
- Training data: finite sequence of pairs that the learner can use.

$$S = ((x_1, y_1), \ldots, (x_m, y_m)) \qquad (x_i, y_i) \in \mathcal{X} \times \mathcal{Y}, \ \forall i$$

Statistical learning framework

- Learner's output $h \in \mathcal{H}$

A model, prediction rule, predictor, hypothesis or classifier.

$$h : \mathcal{X} \to \mathcal{Y}$$

$$x \longrightarrow \boxed{\begin{array}{c}\text{Predictor}\\ h\end{array}} \longrightarrow y$$

Statistical learning framework

Data generation model: $\mathcal{D} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$

The set of all possible probability distributions over domain and target spaces.

Independent and identically distributed (iid)

$$S \sim \mathcal{D}^m$$

$$(x_i, y_i) \sim \mathcal{D}$$

$$P(S) = \prod_{i=1}^{m} P(x_i, y_i)$$

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Statistical learning framework

- Measure of success: loss function

$$l : \underbrace{(\mathcal{X} \times \mathcal{Y})}_{\text{Example}} \times \underbrace{\mathcal{H}}_{\text{Predictor}} \to \underbrace{\mathbb{R}^+}_{\text{Loss}}$$

- Examples:
  - 0/1 loss: $$l_{0-1}((x, y), h) = \begin{cases} 0, & \text{if } h(x) = y \\ 1, & \text{if } h(x) \neq y \end{cases}$$
  - Square loss: $$l_{sq}((x, y), h) := (h(x) - y)^2$$

Definition of risk

$$\underbrace{L_{\mathcal{D}}}_{\text{Data distribution}}\overbrace{(h)}^{\text{Predictor}} := \underbrace{\mathbb{E}_{(x,y)\sim\mathcal{D}}}_{\text{Expectation}}\overbrace{[l((x,y),h)]}^{\text{Loss}}$$

The risk is a weighted sum of the loss where the weight is the probability of the example. However, $\mathcal{D}$ is unknown.

Definition of the empirical risk

$$\underbrace{L_{S}}_{\text{Dataset}}\overbrace{(h)}^{\text{Predictor}} := \underbrace{\frac{1}{m}\sum_{i=1}^{m}}_{\text{Average}}\left[\overbrace{l((x_i, y_i), h)}^{\text{Loss}}\right]$$

The empirical risk is the average of the loss evaluated on our dataset, not all possible examples.

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Empirical risk minimization

Find the predictor that minimizes the empirical risk:

$$h_S = \arg\min_{h \in \mathcal{H}} L_S(h)$$

where

$$L_S(h) := \frac{1}{m} \sum_{i=1}^{m} [l((x_i, y_i), h)]$$

Main question in ML

Will the model perform the same in production than on the training set?

$$L_{\mathcal{D}}(h_S) \overset{?}{\approx} L_S(h_S)$$

where

$$L_{\mathcal{D}}(h) := \boxed{\mathbb{E}_{(x,y)\sim\mathcal{D}}} \left[l((x,y),h) \right]$$

$$L_S(h) := \boxed{\frac{1}{m}\sum_{i=1}^{m}} \left[l((x_i,y_i),h) \right]$$

What can go wrong?

- We only have access to a finite dataset:

$$S = ((x_1, y_1), \ldots, (x_m, y_m)) \qquad\qquad (x_i, y_i) \in \mathcal{X} \times \mathcal{Y},\ \forall i$$

- We are approximating an expectation:

$$L_{\mathcal{D}}(h) := \boxed{\mathbb{E}_{(x,y)\sim\mathcal{D}}} \left[l((x, y), h) \right]$$

$$L_S(h) := \boxed{\frac{1}{m} \sum_{i=1}^{m}} \left[l((x_i, y_i), h) \right]$$

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What can go wrong? Wrong hypothesis class

$$h_S = \arg\min_{h \in \mathcal{H}} L_S(h)$$

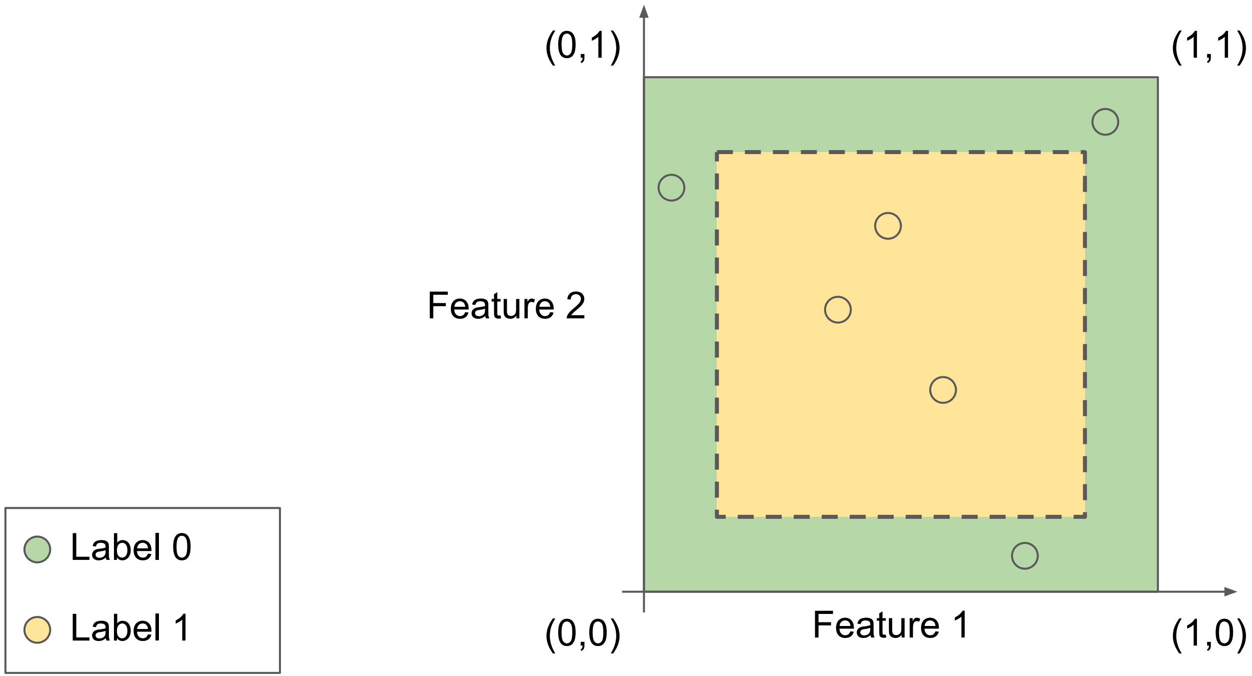
What is the space of predictors?

Optimal predictor for empirical risk: **a lookup table**!

$$h(x) = \begin{cases} y_i, & \text{if } \exists i \text{ st } x = x_i \\ 0, & \text{otherwise} \end{cases}$$

Example: 2D classification problem

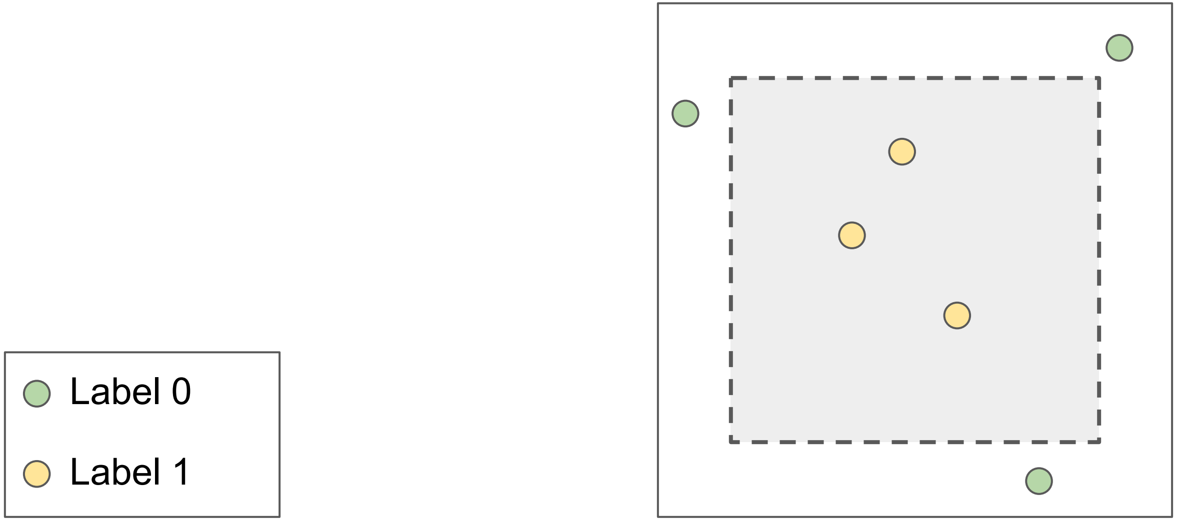
$$\mathcal{D} = \text{Uniform}([0,1]^2)$$



$$l_{0-1}((x,y),h) = \begin{cases} 0, & \text{if } h(x) = y \\ 1, & \text{if } h(x) \neq y \end{cases}$$

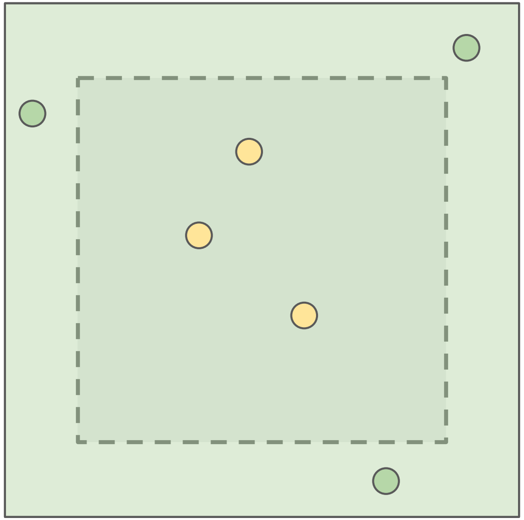
Lookup table predictor

$$h_S(x) = \begin{cases} y_i\,, & \text{if } \exists i \text{ st } x = x_i \\ 0, & \text{otherwise} \end{cases}$$



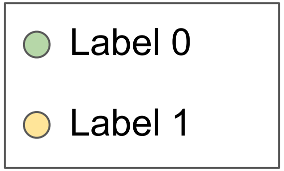
Lookup table predictor: decision boundary

$$h_S(x) = \begin{cases} y_i, & \text{if } \exists i \text{ st } x = x_i \\ 0, & \text{otherwise} \end{cases}$$



$$L_{\mathcal{D}}(h_S) \approx 0.5$$

$$L_S(h_S) = 0$$



What can go wrong? Overfitting

$$\underbrace{L_{\mathcal{D}}}_{\text{Data distribution}}(h_S) \gg \underbrace{L_S}_{\text{Dataset}}\overbrace{(h_S)}^{\text{ERM Predictor}}$$

ERM: Empirical Risk Minimization $\quad h_S = \arg\min_{h \in \mathcal{H}} L_S(h)$

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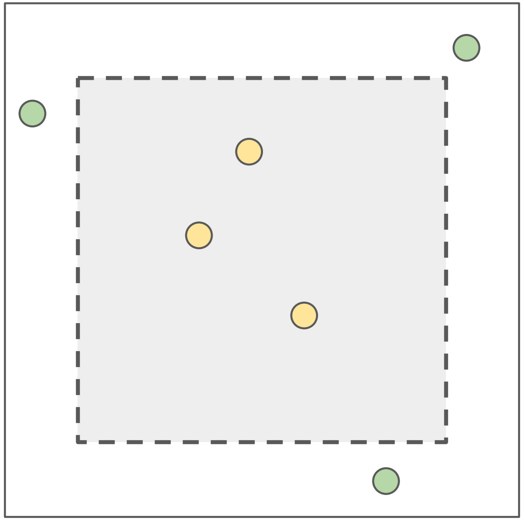
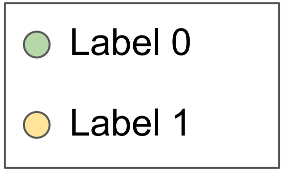
Small improvement: nearest neighbor

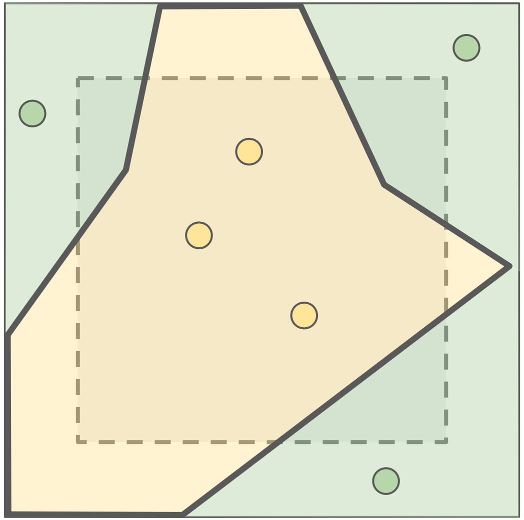
$$h_S(x) = y_i \text{ s.t. } i = \arg\min_i d(x, x_i)$$





Small improvement: nearest neighbor

$$h_S(x) = y_i \text{ s.t. } i = \arg\min_i d(x, x_i)$$



$$L_{\mathcal{D}}(h_S) \approx 0.35$$

$$L_S(h_S) = 0$$

Label 0

Label 1

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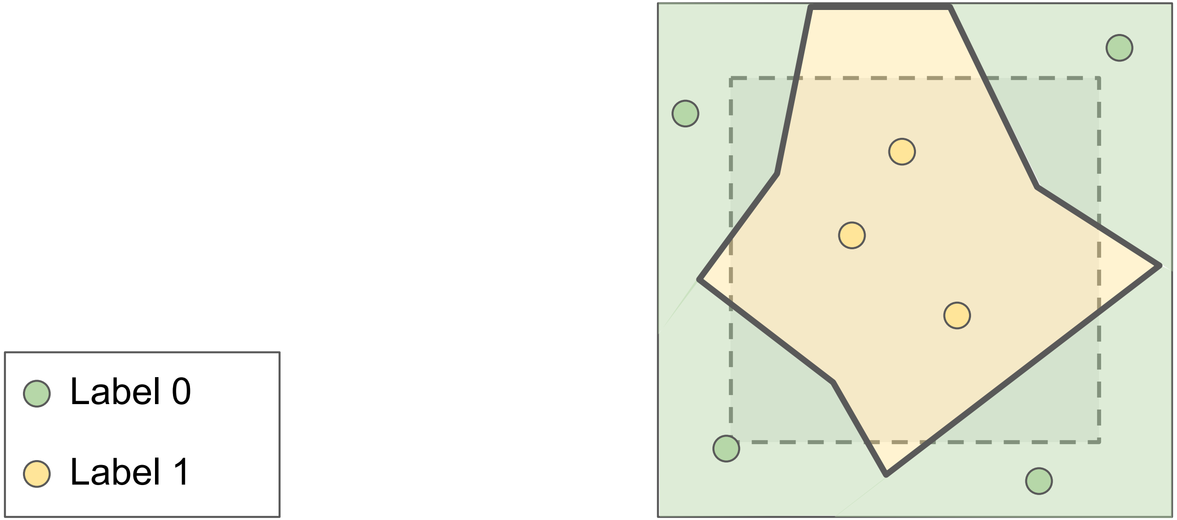
Nearest neighbor: high variance

$$h_S(x) = y_i \text{ s.t. } i = \arg\min_i d(x, x_i)$$



$$L_{\mathcal{D}}(h_S) \approx 0.25$$

$$L_S(h_S) = 0$$

What can go wrong?

- Estimation error: not enough data to estimate risk.
- Wrong hypothesis class: models that can memorize the training dataset or minimize the empirical risk "by chance."

What can go wrong? Wrong hypothesis class

$$h_S = \arg\min_{h \in \mathcal{H}} L_S(h)$$

What is the space of predictors?

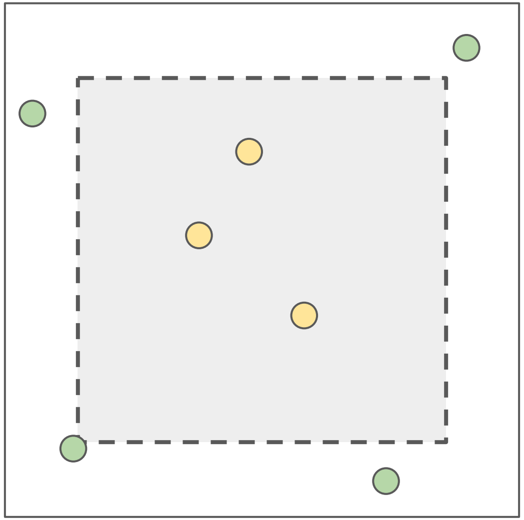
Let $\mathcal{H}$ be the space of linear classifier.

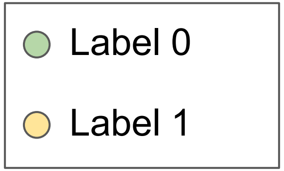
$$h_{w,b}(x) = \mathrm{sign}(\langle w, x \rangle + b)$$

Linear classifier

$$h_{w,b}(x) = \text{sign}(w_1 x_1 + w_2 x_2 + b)$$

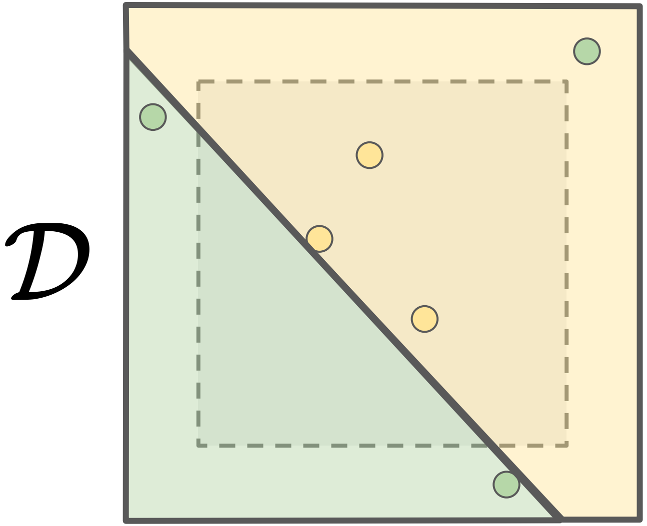
$\mathcal{D}$





Linear classifier

$$h_{w,b}(x) = \mathrm{sign}(w_1 x_1 + w_2 x_2 + b)$$



$$L_{\mathcal{D}}(h_S) \approx 0.70$$

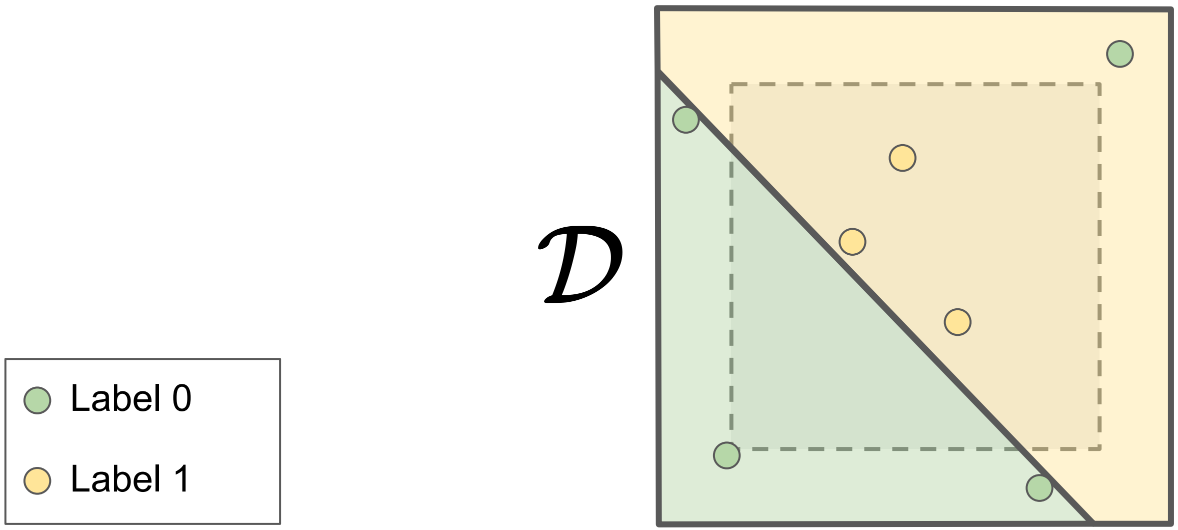
$$L_S(h_S) \approx 0.14$$

Label 0

Label 1

Linear classifier

$$h_{w,b}(x) = \text{sign}(w_1 x_1 + w_2 x_2 + b)$$



$$L_{\mathcal{D}}(h_S) \approx 0.70$$

$$L_S(h_S) \approx 0.14$$

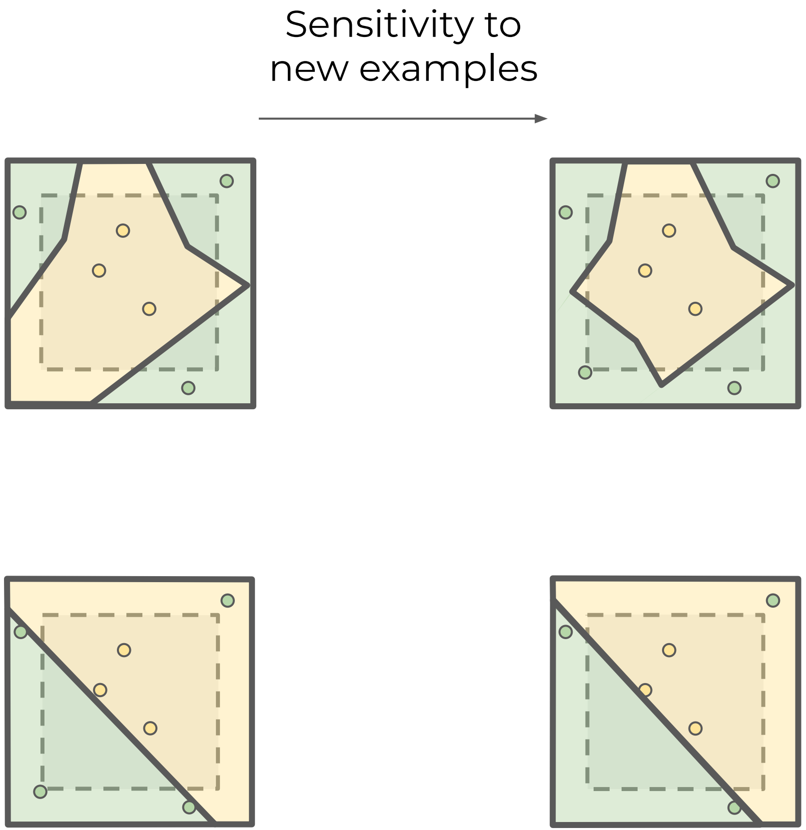
Two different hypothesis classes

- Class of nearest neighbor classifiers
    - Instance-based learning (all the dataset is kept in memory).
    - Decision boundaries are complex and sensitive to new examples.
- Class of linear classifiers
    - Parametric model.
    - Decision boundaries are simple, and robust to new examples.

Bias vs. variance

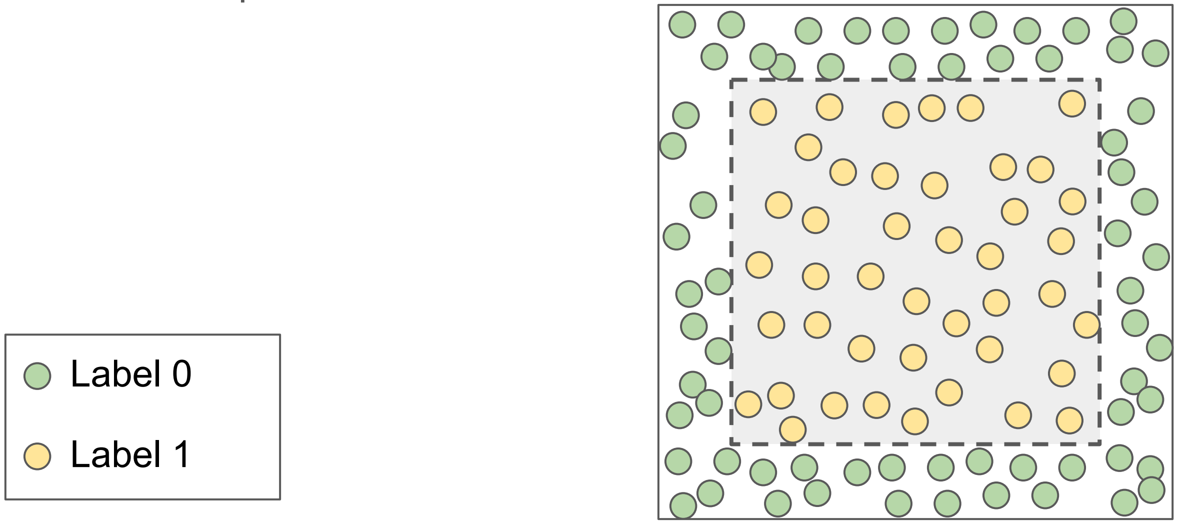
Estimation error
(High variance)

Approximation error
(High bias)



Can more data be the solution?

- Theoretically Yes! By using the nearest neighbor algorithm with a large number of examples, the empirical risk minimizer will be close to the best predictor.



Can more data be the solution?

In practice, **No**! The number of examples to cover the domain space $\mathcal{X}$ grows too fast with respect to the dimension of $\mathcal{X}$.

Data is **necessary**, but **not sufficient**.

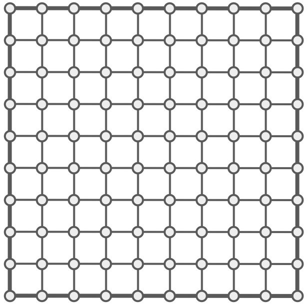
Can more data be the solution?

Intuition: suppose $\mathcal{X} = [0,1]^d$, we want to cover $\mathcal{X}$ with precision $\epsilon = 0.1$, i.e., the **largest distance** between two points x_i, x_j.

$d = 1$

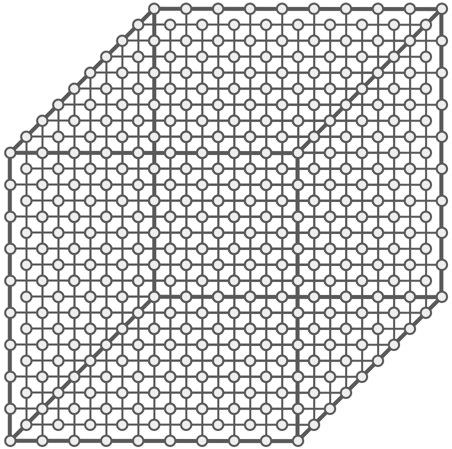
$m = 10$

$d = 2$



$m = 100$

$d = 3$



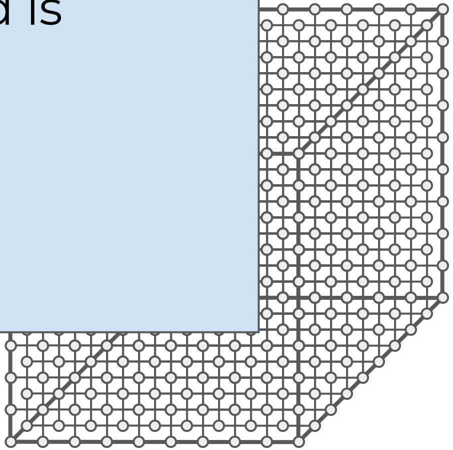
$m = 1000$

Can more data be the solution?

Intuition: suppose $\mathcal{X} = [0,1]^d$, we want to cover $\mathcal{X}$ with precision $\epsilon = 0.1$, i.e., the **largest distance** between two points x_i, x_j .

$d = 1$

3



The number of examples required is **exponential** in the dimension.

$$\epsilon^{-d}$$

$m = 10$ $m = 100$ $m = 1000$

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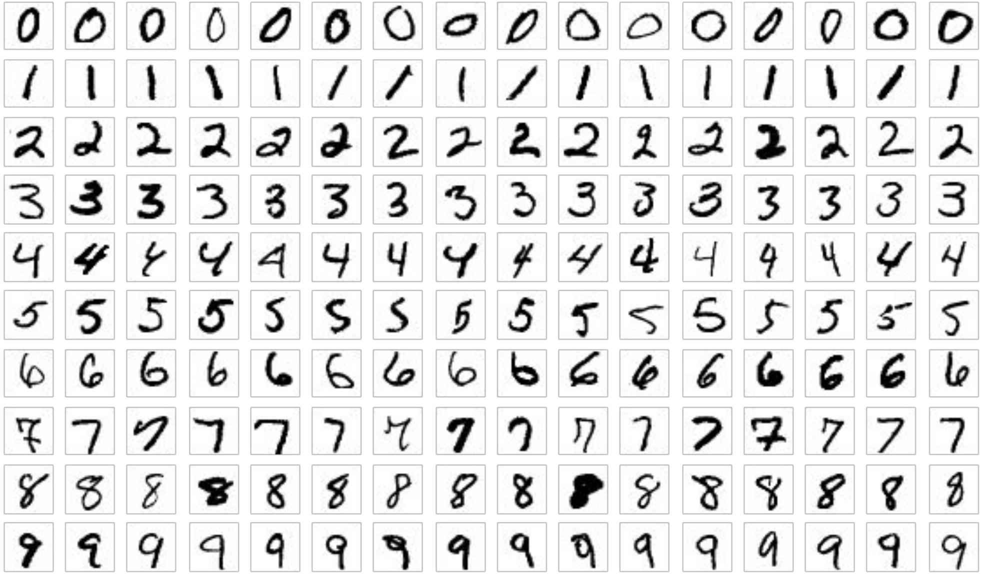
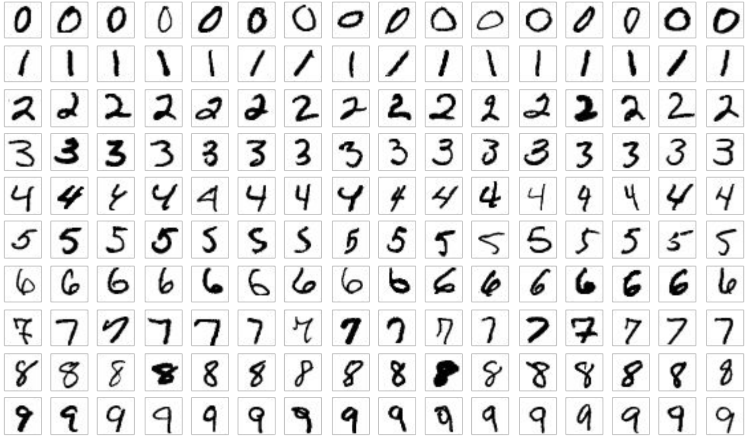
Simple example: MNIST

Image classification: image size 28x28=784. $0.1^{-784} = 10^{784}$ examples!



Simple example: MNIST

If we sample uniformly from $\mathcal{X} = [0, 1]^{784}$, the probability of obtaining a digit is close to 0. In high dimension, we have that each example is far from others.



Manifold assumption

In high-dimension, a lower-dimensional manifold supports the data distribution. The data **representation** has too many degrees of freedom compared to the underlying system.

The underlying system has 43 degrees of freedom (facial muscles) + some deformable parts (glasses, hair, ...)

The image representation has 960x720x3=2,073,600 degrees of freedom (RGB pixels).

What is the best hypothesis class?

$$h_S = \arg\min_{h \in \mathcal{H}} L_S(h)$$

Inductive bias

We choose the hypothesis class and how to navigate in it with our prior knowledge on the task.

ML/DL expertise

$$h_S = \arg\min_{h \in \mathcal{H}} L_S(h)$$

What is the space of predictors?

This is why you are attending this deep learning school!

How to choose $\mathcal{H}$?

- **Deep learning** is a powerful way to describe parametric models in terms of computational modules.
- We use an iterative algorithm to change the model parameters in order to reduce the empirical risk.
- We can also restrict the values taken by the parameters in order to reduce the complexity of $\mathcal{H}$. We call this restriction **regularization**.

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Hyperparameter tuning

and model selection

How to diagnose overfitting?

Can we detect when

$$L_{\mathcal{D}}(h_S) \gg L_S(h_S) \text{ ?}$$

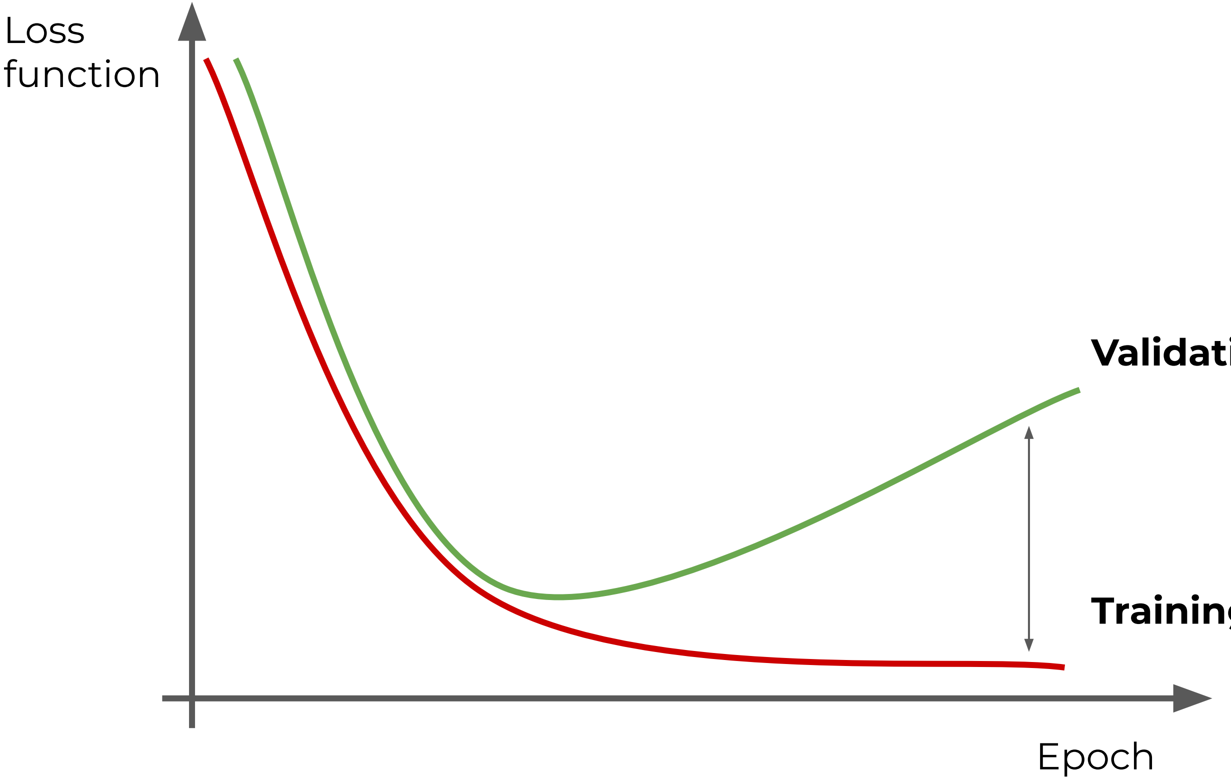
Hold out method (Validation set)

Monitor the loss function on **an independent set** of examples.

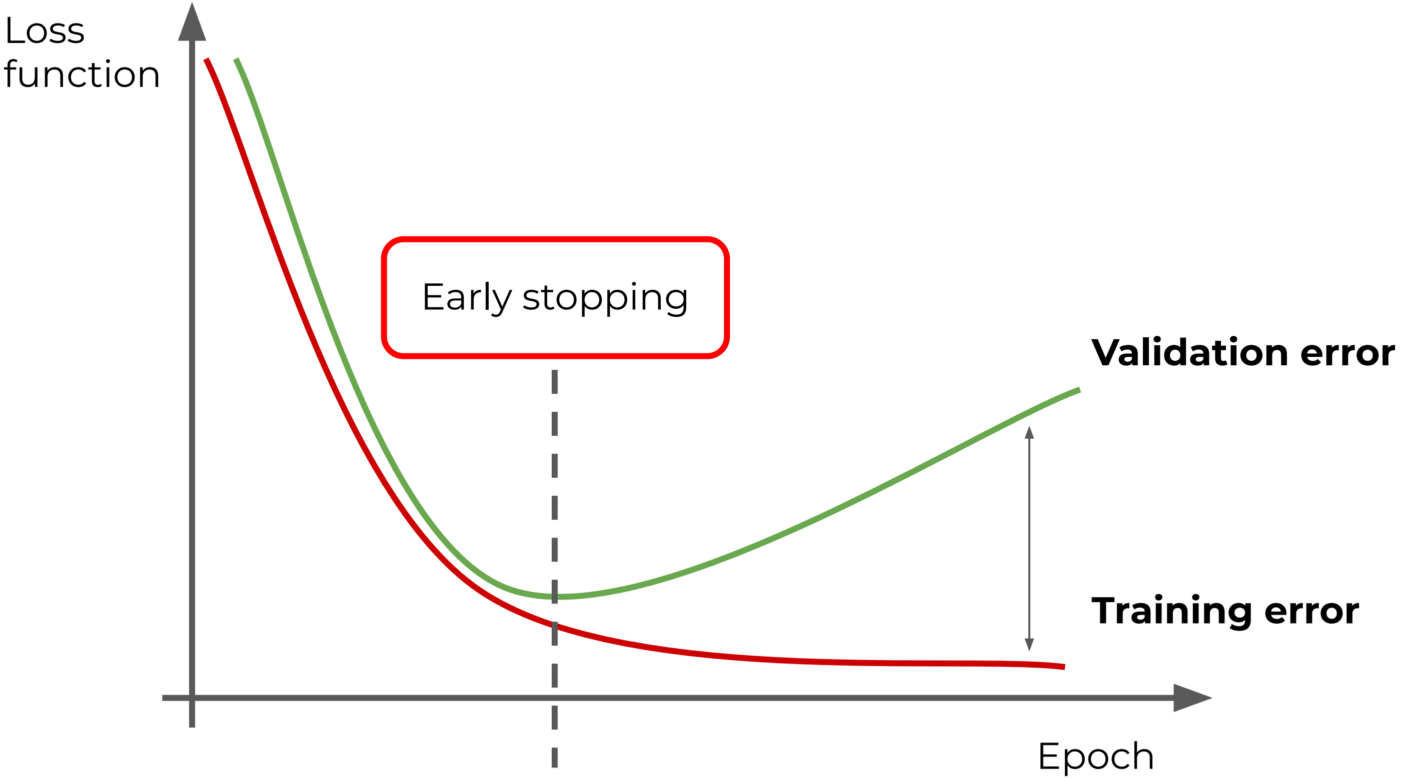
$$V = ((x_1, y_1), \ldots, (x_{m_v}, y_{m_v})) \qquad (x_i, y_i) \sim \mathcal{D}$$

$$L_V(h) := \frac{1}{m_v} \sum_{i=1}^{m_v} [l((x_i, y_i), h)]$$

How to diagnose overfitting?

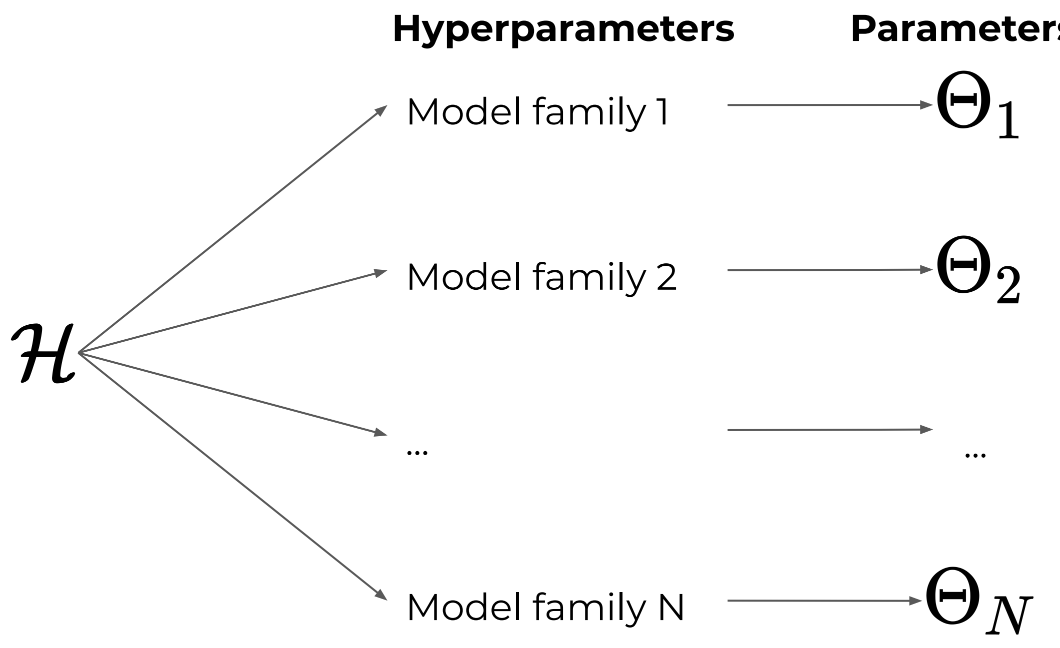


How to diagnose overfitting?



Hyperparameters tuning and model selection

$\mathcal{H}$ can have a complex structure.



Each model family has its own parameter space and optimization algorithm.

Hyperparameters tuning and model selection

Find the model with minimal risk for each family with **the training set**.

	Hyperparameters		ERM Predictors
$\mathcal{H}$ $\rightarrow$	Model family 1	$\longrightarrow$	h_S^1
$\mathcal{H}$ $\rightarrow$	Model family 2	$\longrightarrow$	h_S^2
$\mathcal{H}$ $\rightarrow$	…	$\longrightarrow$	…
$\mathcal{H}$ $\rightarrow$	Model family N	$\longrightarrow$	h_S^N

Hyperparameters tuning and model selection

Evaluate the ERM predictors on **the validation set**.

	Hyperparameters	ERM Predictors	Validation
$\mathcal{H}$	Model family 1	h_S^1	$L_V(h_S^1)$
	Model family 2	h_S^2	$L_V(h_S^2)$
	...	...	...
	Model family N	h_S^N	$L_V(h_S^N)$

Hyperparameters tuning and model selection

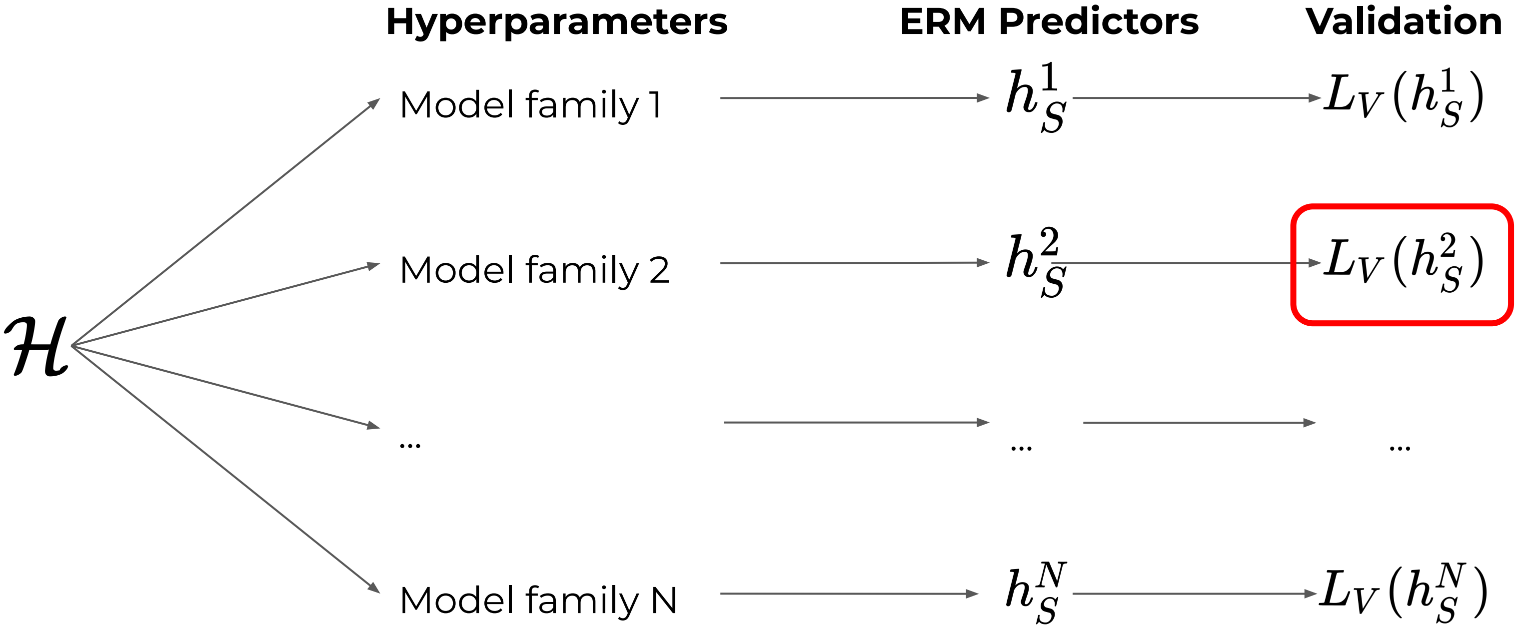
Choose the predictor with the lowest risk on the validation set.

$\mathcal{H}$

Hyperparameters	ERM Predictors	Validation
Model family 1	h_S^1	$L_V(h_S^1)$
Model family 2	h_S^2	$\boxed{L_V(h_S^2)}$
...	...	...
Model family N	h_S^N	$L_V(h_S^N)$

Test set

If the number of model families is high, we can **overfit the validation set**.



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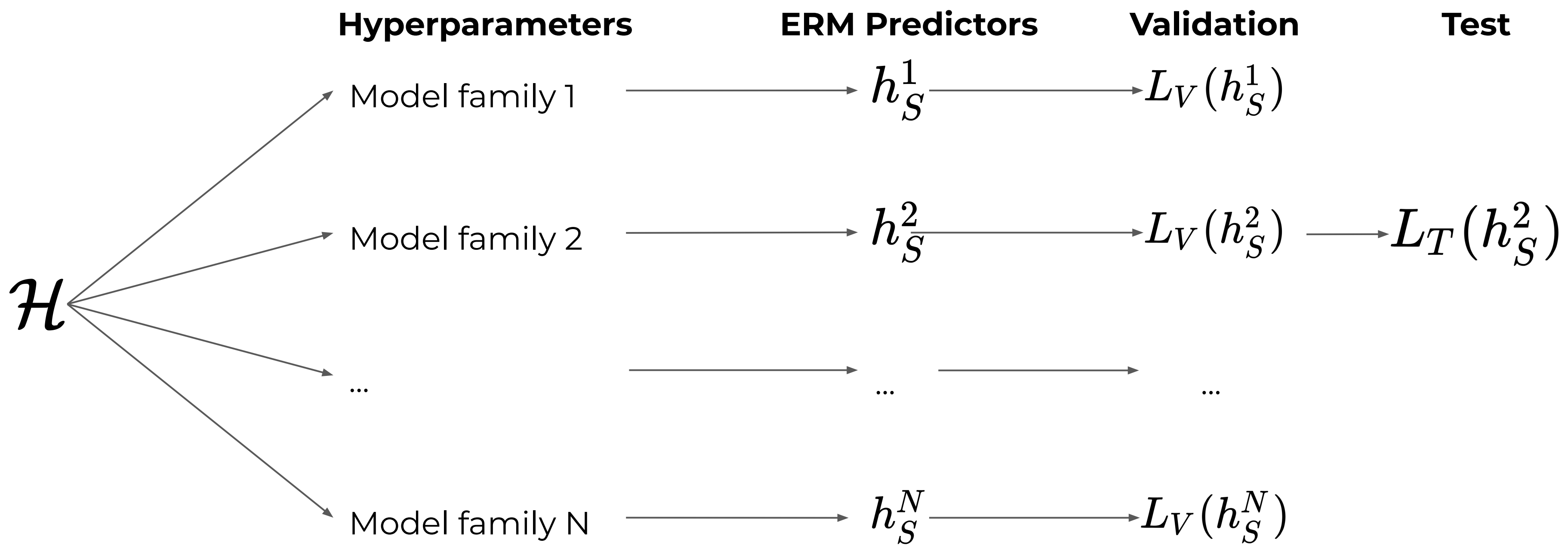
Test set

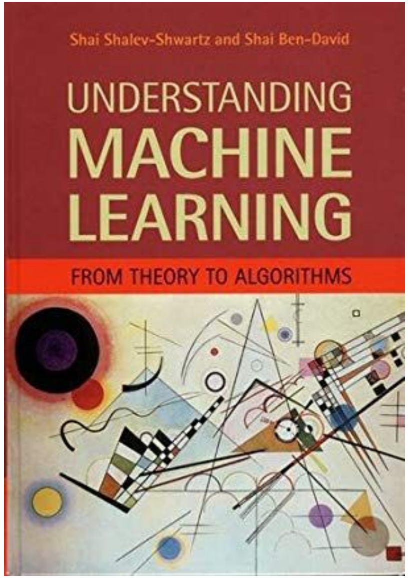
So, we use another set called the **test set** T .



Take-home message

- Different types of learning have been studied in the literature.
- Statistical learning framework helps us to understand overfitting.
- Models can be too biased or have too much variance.
- Data is necessary, but not sufficient.
- Deep learning is an efficient way to define hypothesis classes.

References


Shai Shalev-Shwartz and Shai Ben-David
UNDERSTANDING
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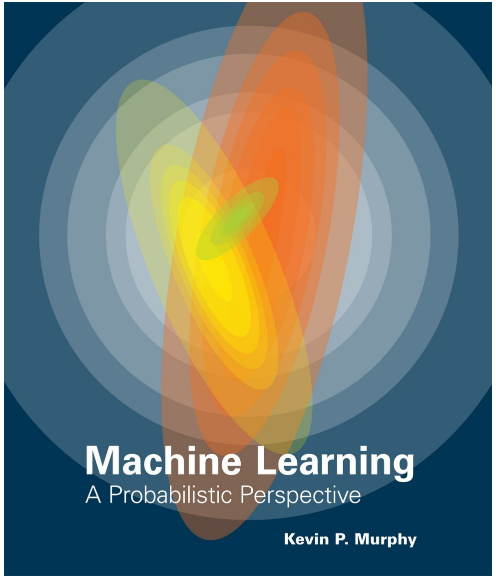
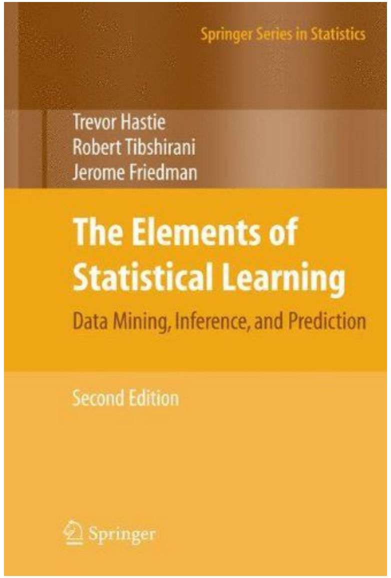
FROM THEORY TO ALGORITHMS


Machine Learning
A Probabilistic Perspective
Kevin P. Murphy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