CSC 480/580 Principles of Machine Learning

02 Limits of Learning

Chicheng Zhang

Department of Computer Science

The University of Arizona

Motivation

- Supervised learning is a general & useful framework

- Understand when supervised learning will and will not work

Bayes optimal classifier and its error

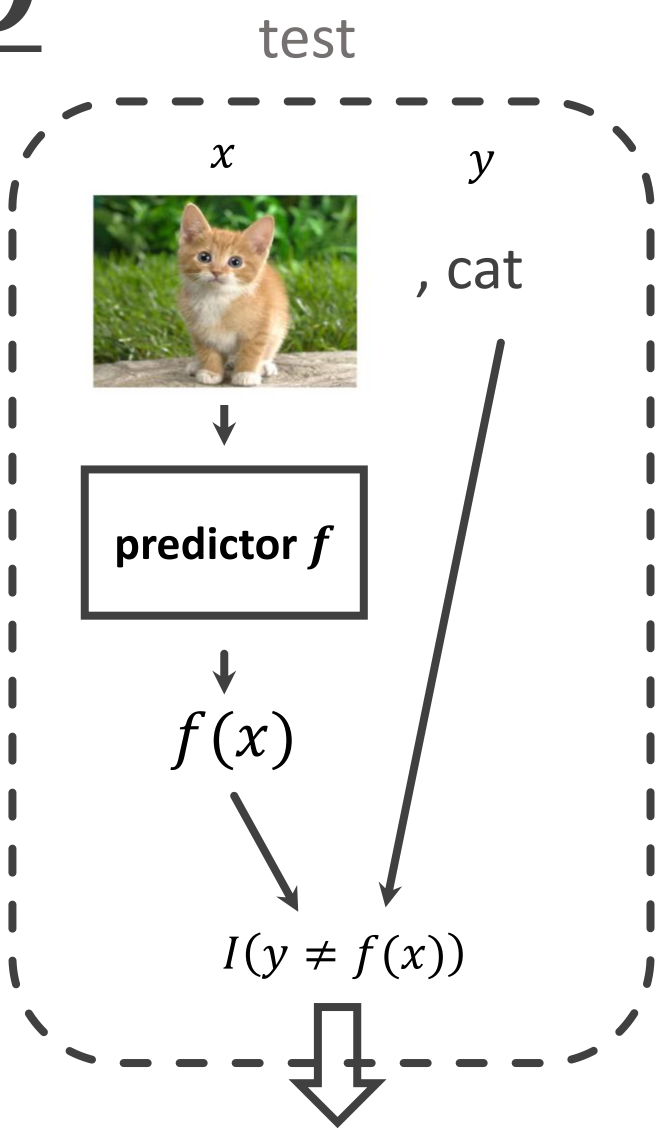
Optimal classification with **known *D***

- Suppose: $I(A) = 1$ *if A happens, and = 0 otherwise*
  - Binary classification, 0-1 loss $\ell(y, \hat{y}) = I(y \neq \hat{y})$
  - D is *known:* for every (x, y), $P_D(x, y)$ is known to us

- What is the f that has the smallest *generalization error*

  $L_D(f) = \mathrm{E}_{(x,y)\sim D} I(y \neq f(x))$?

- Note (alternative expression) : $L_D(f) = P_{(x,y)\sim D}\ (y \neq f(x))$



Generalization error: $L_D(f)$ = $\mathrm{E}_{(x,y)\sim D} I(y \neq f(x))$

Simple case: discrete domain $\mathcal{X}$

- Predicting whether the student will pass the course (y), given her project grade (x)

$P_D(x,y)$	$x=1$	$x=2$	$x=3$
$y=-1$	0.2	0.2	0.15
$y=+1$	0.1	0.3	0.05

Which classifier is better?

- $f_1(1)=-1, f_1(2)=-1, f_1(3)=-1 \quad \Rightarrow \quad L_D(f_1)=0.1+0.3+0.05$
- $f_2(1)=-1, f_2(2)=+1, f_2(3)=-1 \quad \Rightarrow \quad L_D(f_2)=0.1+0.2+0.05$

Is this the best classifier? Why?

- For any x, should predict y that has higher value of $P_D(x,y)$
- Intuition: predict the label that **better correlates** with the feature x
- $f^*(1)=-1, f^*(2)=+1, f^*(3)=-1$

Bayes optimal (BO) classifier

Theorem f_{BO} achieves the smallest generalization error among all classifiers.

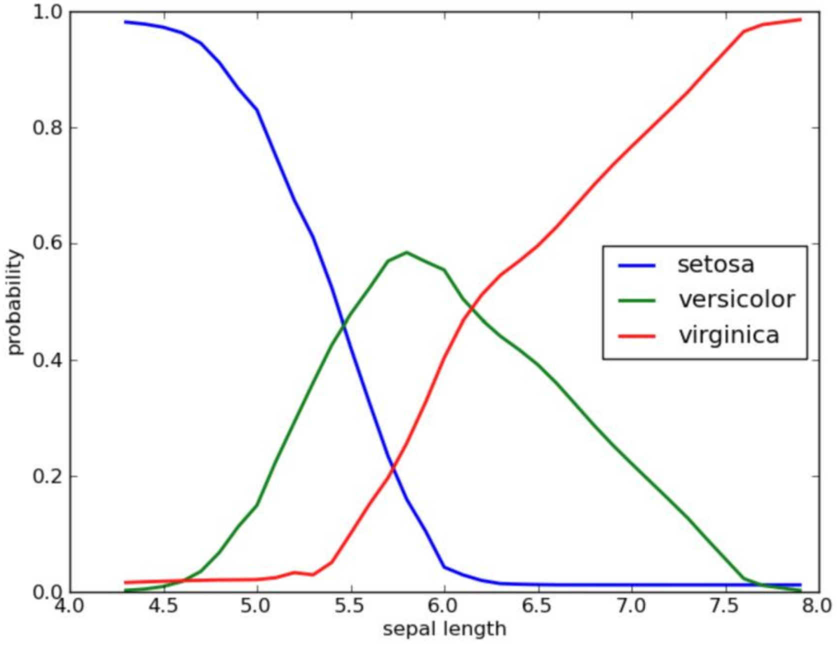
$$f_{BO}(x) = \arg\max_{y \in \mathcal{Y}} P_D(X = x, Y = y) = \arg\max_{y \in \mathcal{Y}} P_D(Y = y \,|X = x)\,, \forall x \in \mathcal{X}$$

Example Iris dataset classification:

Iris Setosa

Iris Versicolor

Iris Virginica



Proof of theorem

Step 1 consider accuracy,

- $A_D(f) = 1 - L_D(f) = P_D\big(Y = f(X)\big) = \sum_x P_D\big(X = x, Y = f(x)\big)$
- Suffices to show f_{BO} has the highest accuracy

Step 2 comparison,

$$A_D(f_{BO}) - A_D(f) = \sum_x P_D\big(X = x, Y = f_{BO}(x)\big) - P_D\big(X = x, Y = f(x)\big) \geq 0$$

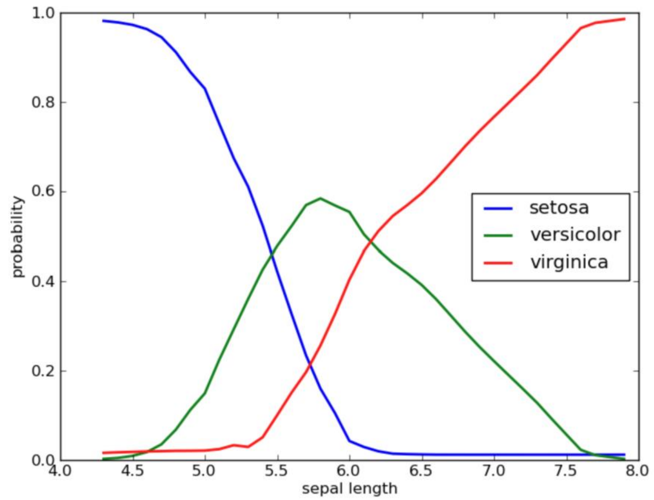
$$\boxed{f_{BO}(x) = \arg\max_{y \in \mathcal{Y}} P_D(X = x, Y = y)}$$

Remarks

- Similar reasoning can be used to prove the theorem with continuous domain $\mathcal{X}$ (sum -> integral)
- This just shows deterministic classifier, can be extended to show BO is 0-1 optimal for all classifiers

Bayes error rate: alternative form

$$
\begin{aligned}
L_D(f_{BO}) &= P_D\big(Y \neq f_{BO}(X)\big) \\
&= \textstyle\sum_x P_D(Y \neq f_{BO}(x) \mid X = x)\, P_D(X = x) \\
&= \textstyle\sum_x (1 - P_D(Y = f_{BO}(x) \mid X = x))\, P_D(X = x) \\
&= \textstyle\sum_x \left(1 - \max\limits_y P_D(Y = y \mid X = x)\right) P_D(X = x) \\
&= \mathrm{E}\left[1 - \max\limits_y P_D(Y = y \mid X)\right]
\end{aligned}
$$



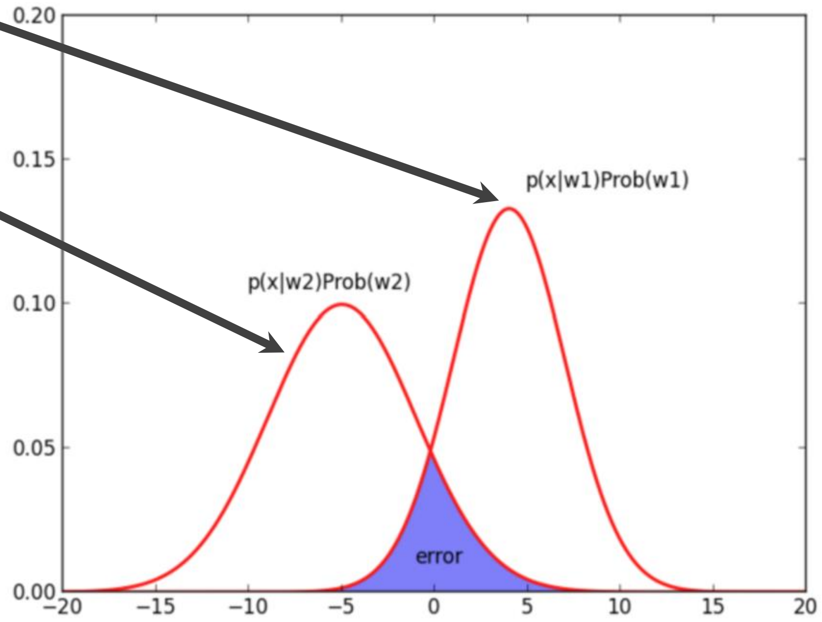
Bayes error rate: binary classification case

- $L_D(f_{BD}) = \mathrm{E}\left[1 - \max_y P_D(Y = y \mid X)\right]$

$$= \mathrm{E}\left[\min_y P_D(Y = y \mid X)\right]$$

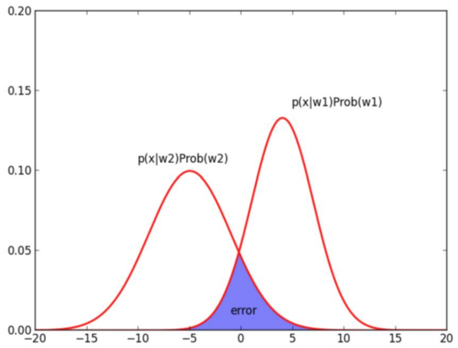
$$= \sum_x \min(\, P_D(Y = +1, X = x)\,, P_D(Y = -1, X = x))$$

$P_D(x, y)$	$x = 1$	$x = 2$	$x = 3$
$y = -1$	0.2	0.2	0.15
$y = +1$	0.1	0.3	0.05



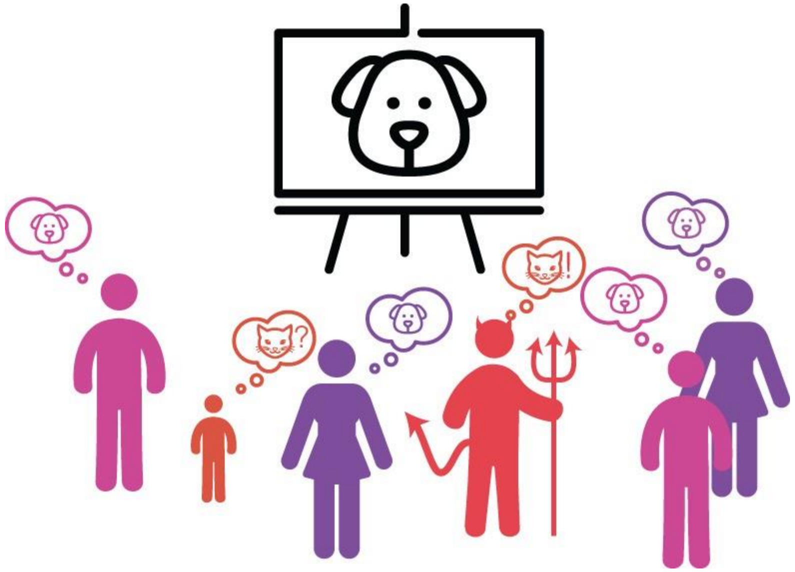
- Note: the Bayes error rate is a property of data distribution D
- Q: for a distribution D, when is its Bayes error rate zero?

When is the Bayes error rate nonzero?



- $L_D(f_{BO}) = 0$ if y is **deterministic** given x (for $(x, y) \sim D$)
- $L_D(f_{BO}) \neq 0$ if $y \mid x$ is not deterministic for some x

- $L_D(f_{BO}) \neq 0$ when we have:
- Limited feature representation (e.g. predicting gender using only height)
- Noise in the data
  - Feature noise – e.g. Sensor failure, Typo in reviews for sentiment classification
  - Label noise – e.g. typo transcribing reviews
- May not have a single “correct” label

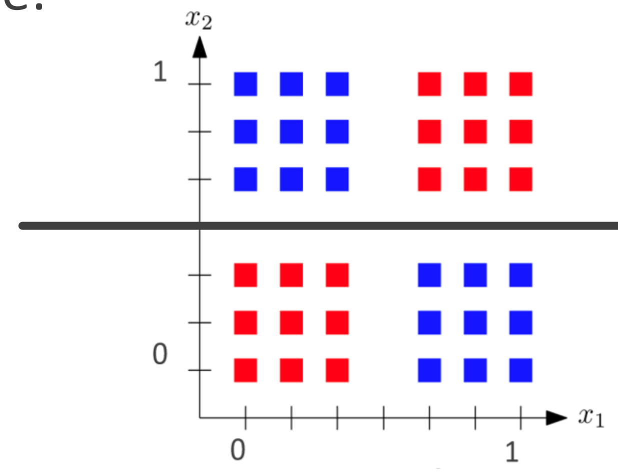


Overfitting: when does it happen and how to detect it

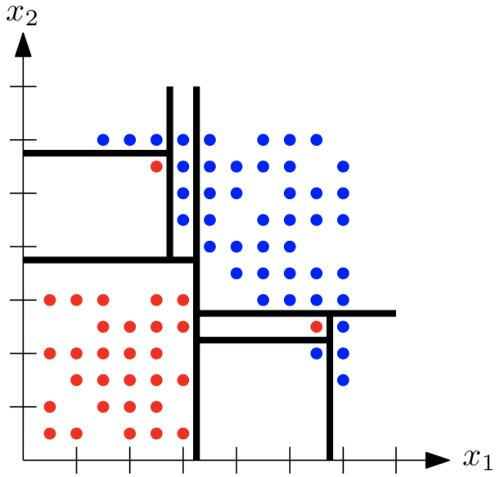
Overfitting vs Underfitting

- Q: should I train a shallow or deep decision tree?

- Shallow tree:

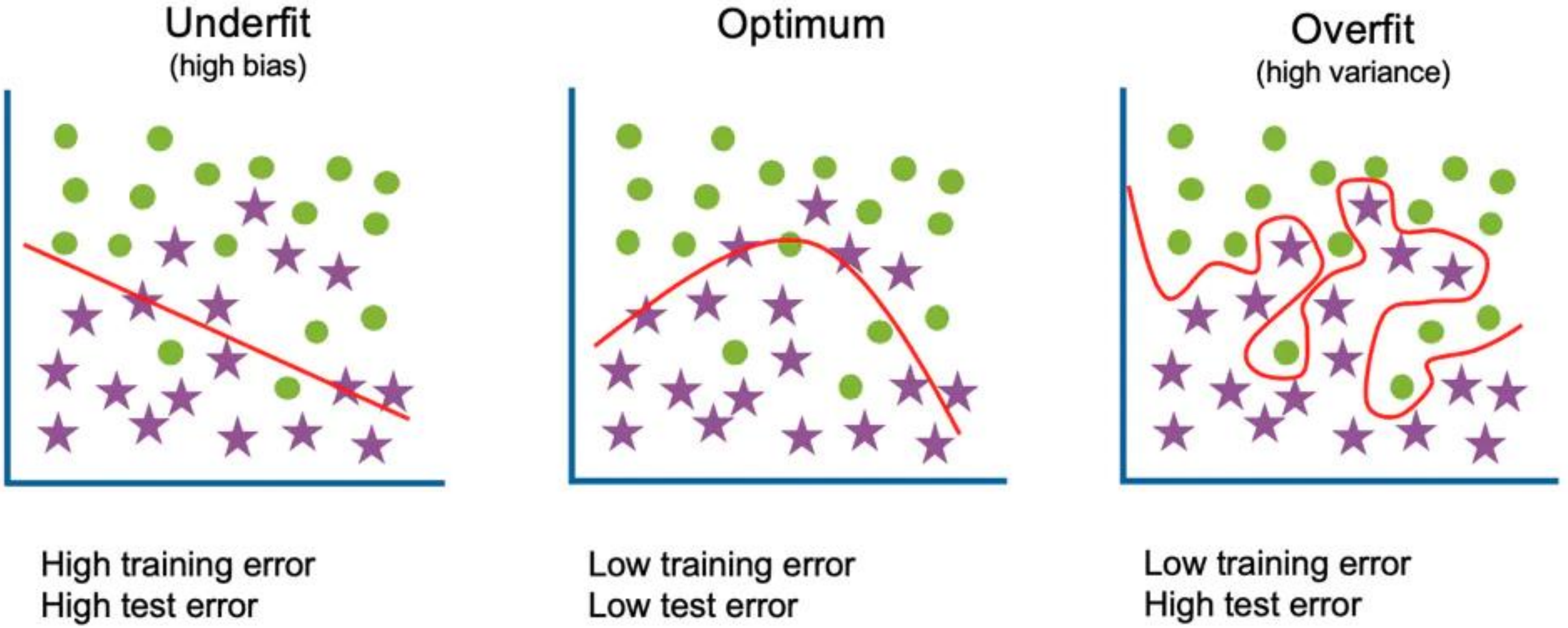


Deep tree:



- Underfitting: have the opportunity to learn something but didn't
- Overfitting: pay too much attention to idiosyncrasies to training data, and do not generalize well
- A model that neither overfits nor underfits is expected to do best

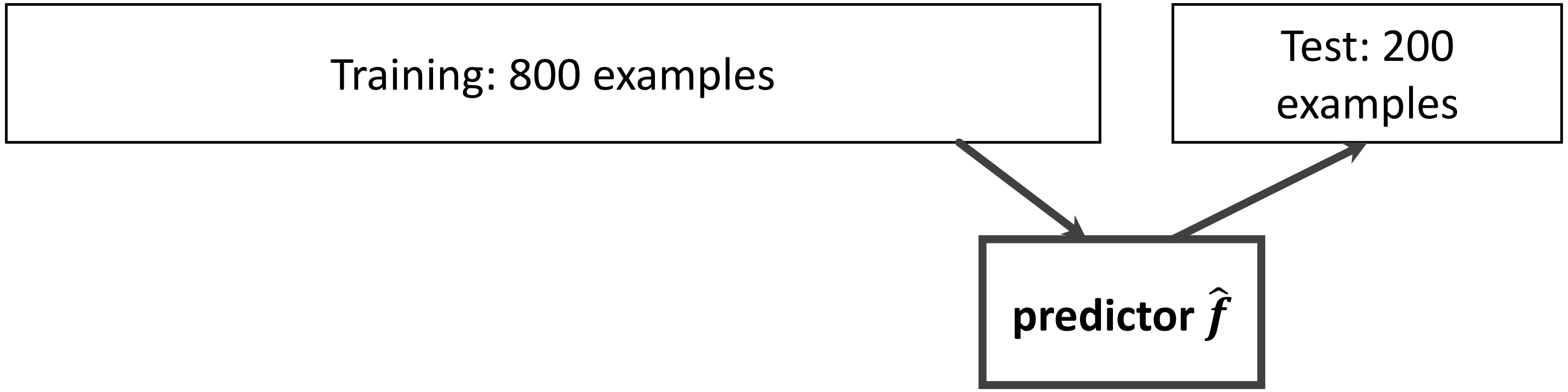
Overfitting vs Underfitting



Source: ibm.com

Unbiased model evaluation using test data

- Your boss says: I will allow your recommendation system to run on our website only if the error is <= 10%!
- How to prove it?
- Idea: reserve some data as test data for evaluating predictors

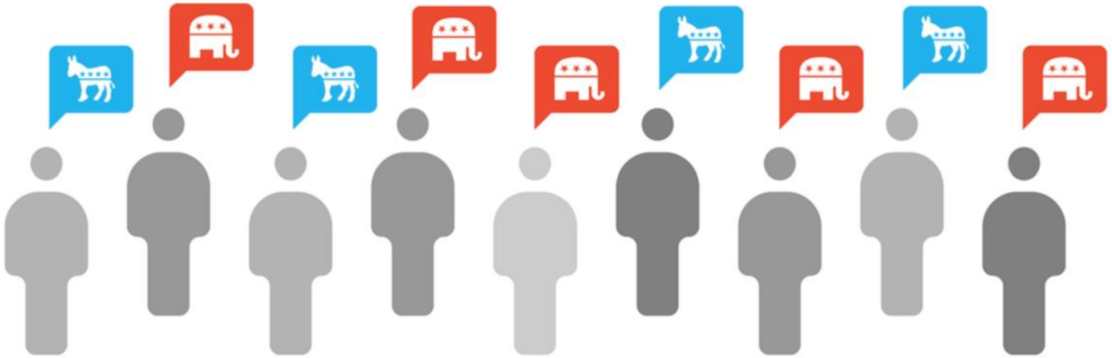


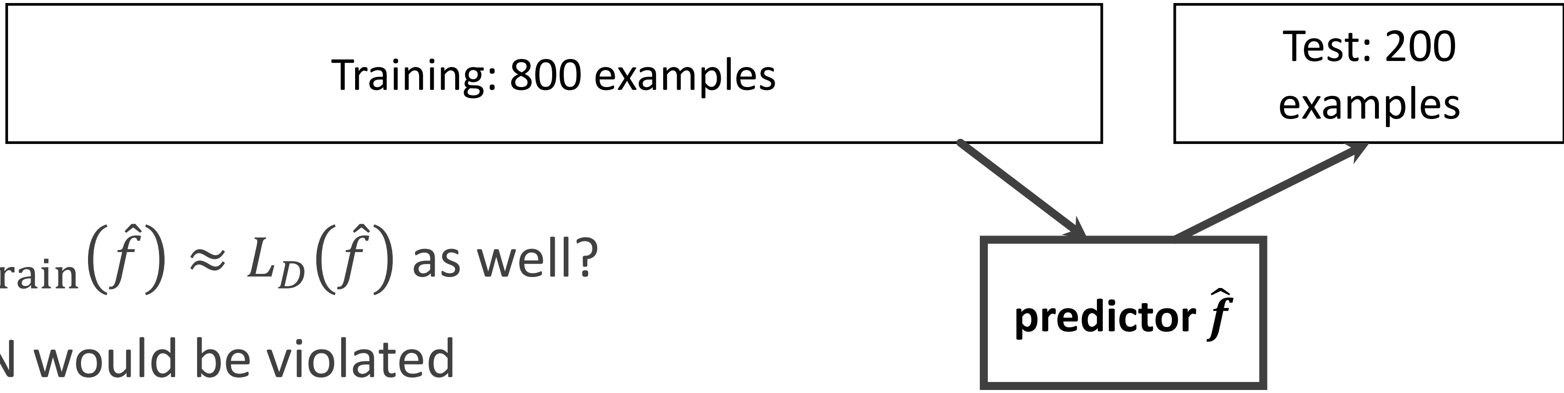
- Justification:
- $L_{\text{test}}(\hat{f}) = \frac{1}{|S_{\text{test}}|} \sum_{(x,y) \in S_{\text{test}}} I(y \neq \hat{f}(x))$
- Law of large numbers $\Rightarrow L_{\text{test}}(\hat{f}) \to L_D(\hat{f})$

Law of large numbers (LLN)

- Suppose $v_1, \dots, v_n$ are IID (independent & identically distributed) random variables, the sample average $\bar{v} = \frac{1}{n}\sum_{i=1}^{n} v_i$ converges to $\mathrm{E}[v_1]$ as $n \to \infty$

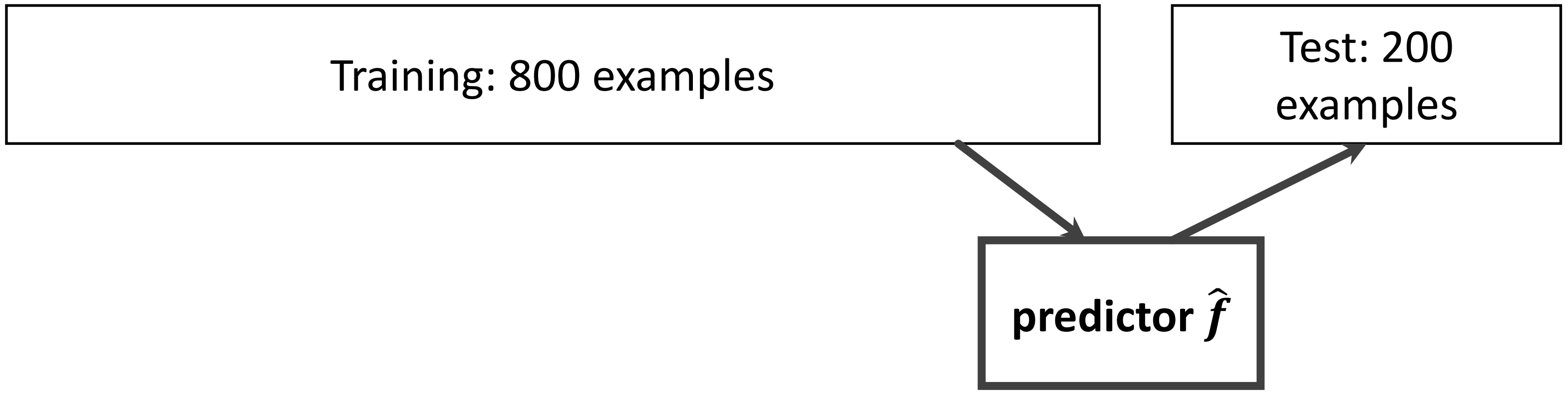
- Useful in e.g. election poll
- Cornerstone of statistics





- LLN justifies that $L_{\text{test}}(\hat{f}) \approx L_D(\hat{f})$
- Can we apply LLN to conclude that $L_{\text{train}}(\hat{f}) \approx L_D(\hat{f})$ as well?
- **No!** The IID condition for applying LLN would be violated

Never touch your test data!



- More precisely: test data should be used **<u>only once</u>** for final evaluation
- Otherwise, $\hat{f}$ depends on test examples, $L_{\text{test}}(\hat{f}) \approx L_D(\hat{f})$ may no longer be true
- Be mindful about indirect dependence as well:
  - adaptive data analysis – after seeing a previous algorithm doing badly on test data, develop a new learning algorithm that produces $\hat{f}$

Case Study: MNIST Dataset

All publications use standard train/test split

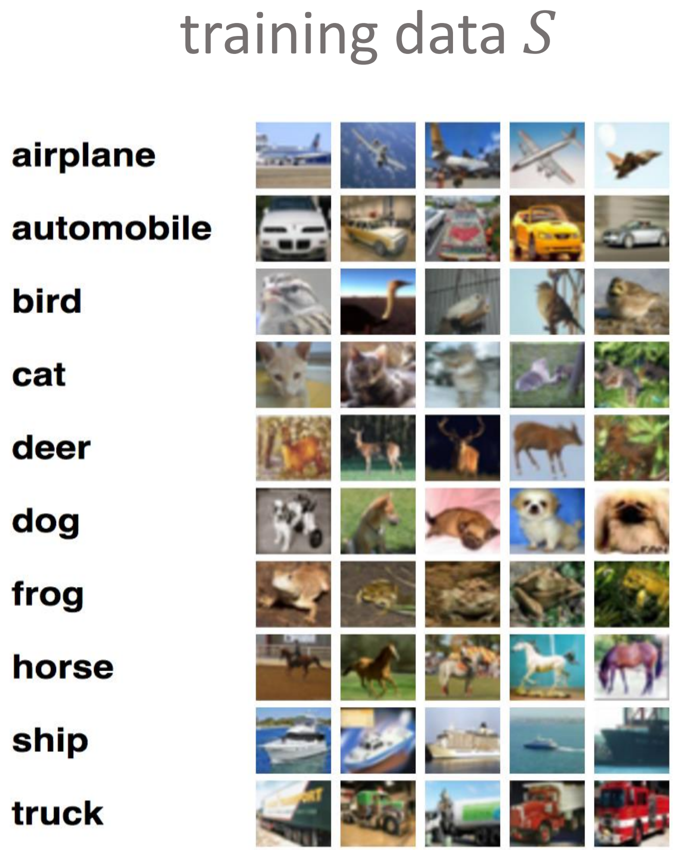
Hundreds of publications compare to each other

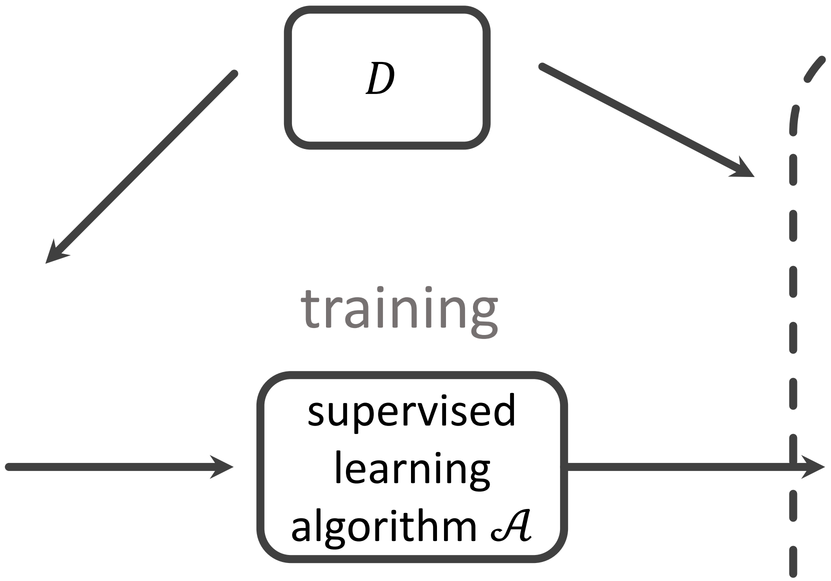
Type	Classifier	Distortion	Preprocessing	Error rate (%)
Linear classifier	Pairwise linear classifier	None	Deskewing	7.6[10]
Decision stream with Extremely randomized trees	Single model (depth > 400 levels)	None	None	2.7[28]
K-Nearest Neighbors	K-NN with rigid transformations	None	None	0.96[29]
K-Nearest Neighbors	K-NN with non-linear deformation (P2DHMDM)	None	Shiftable edges	0.52[30]
Boosted Stumps	Product of stumps on Haar features	None	Haar features	0.87[31]
Non-linear classifier	40 PCA + quadratic classifier	None	None	3.3[10]
Random Forest	Fast Unified Random Forests for Survival, Regression, and Classification (RF-SRC)[32]	None	Simple statistical pixel importance	2.8[33]
Support-vector machine (SVM)	Virtual SVM, deg-9 poly, 2-pixel jittered	None	Deskewing	0.56[34]
Deep neural network (DNN)	2-layer 784-800-10	None	None	1.6[35]
Deep neural network	2-layer 784-800-10	Elastic distortions	None	0.7[35]
Deep neural network	6-layer 784-2500-2000-1500-1000-500-10	Elastic distortions	None	0.35[36]
Convolutional neural network (CNN)	6-layer 784-40-80-500-1000-2000-10	None	Expansion of the training data	0.31[37]
Convolutional neural network	6-layer 784-50-100-500-1000-10-10	None	Expansion of the training data	0.27[38]
Convolutional neural network (CNN)	13-layer 64-128(5x)-256(3x)-512-2048-256-256-10	None	None	0.25[22]
Convolutional neural network	Committee of 35 CNNs, 1-20-P-40-P-150-10	Elastic distortions	Width normalizations	0.23[17]
Convolutional neural network	Committee of 5 CNNs, 6-layer 784-50-100-500-1000-10-10	None	Expansion of the training data	0.21[24][25]
Random Multimodel Deep Learning (RMDL)	10 NN-10 RNN - 10 CNN	None	None	0.18[27]
Convolutional neural network	Committee of 20 CNNS with Squeeze-and-Excitation Networks[39]	None	Data augmentation	0.17[40]
Convolutional neural network	Ensemble of 3 CNNs with varying kernel sizes	None	Data augmentation consisting of rotation and translation	0.09[41]

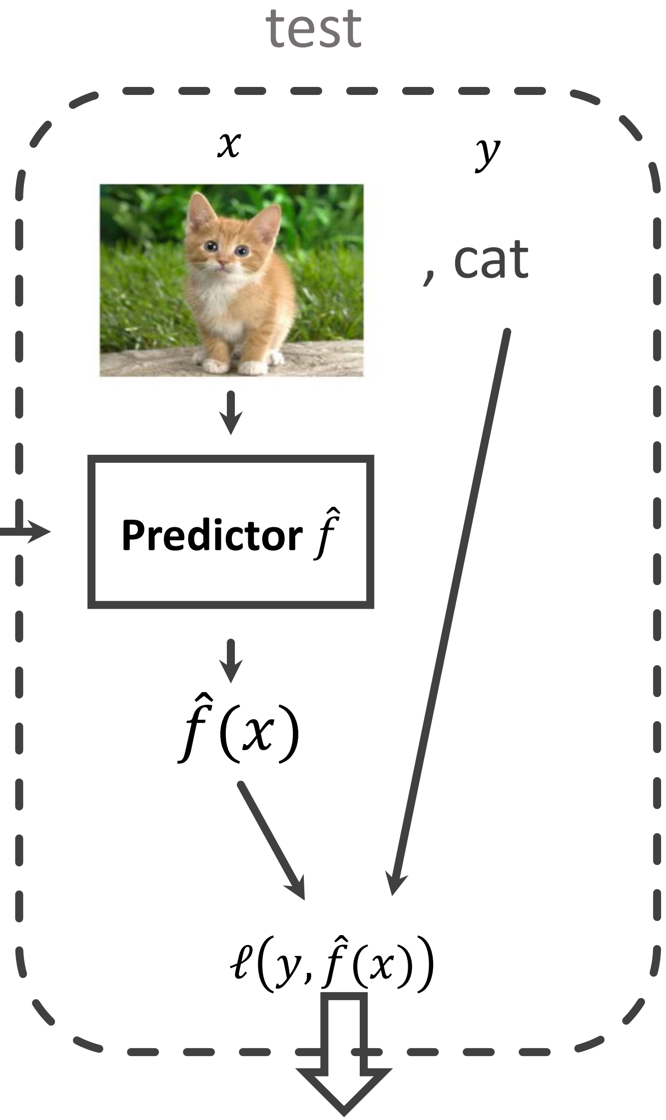
What's the problem with this?

Combatting overfitting via hyperparameter tuning (aka model selection)

Supervised learning setup





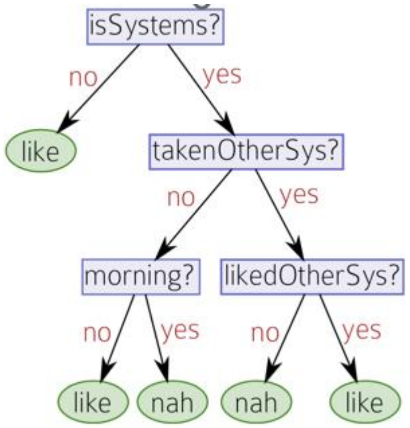


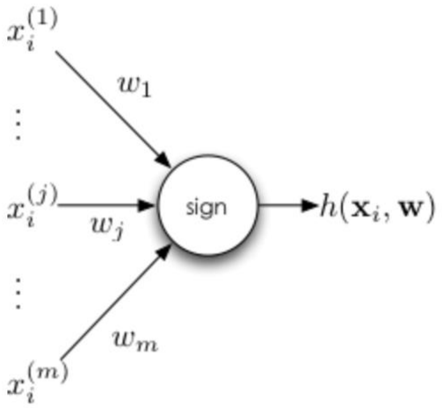
- Goal: design learning algorithm $\mathcal{A}$ such that its output $\hat{f}$ on iid training data S has low generalization error

Generalization error: $L_D(\hat{f}) = \mathrm{E}_{(x,y)\sim D}\, \ell(y, \hat{f}(x))$

Terminologies

- **Model:** the predictor $\hat{f}$
  - Often from a model class (family) $\mathcal{F}$,
  - e.g. $\mathcal{F} = \{\text{depth} - 5 \text{ decision trees}\}, \{\text{linear classifiers}\}$





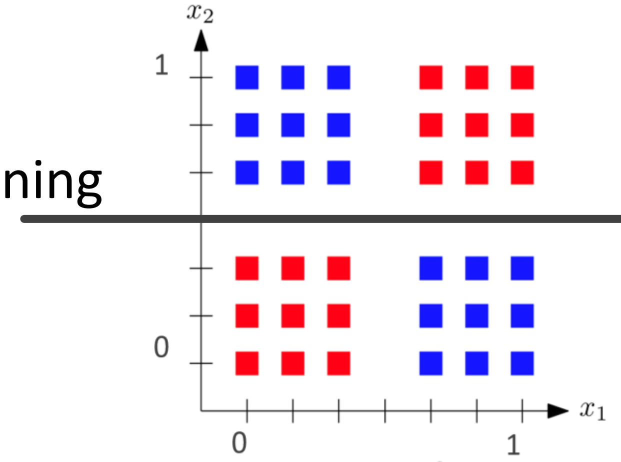
- **Parameter:** specifics of $\hat{f}$
  - E.g. for decision tree $\hat{f}$: tree structure, questions in nodes, labels in leaves
  - For linear classifier: linear coefficients

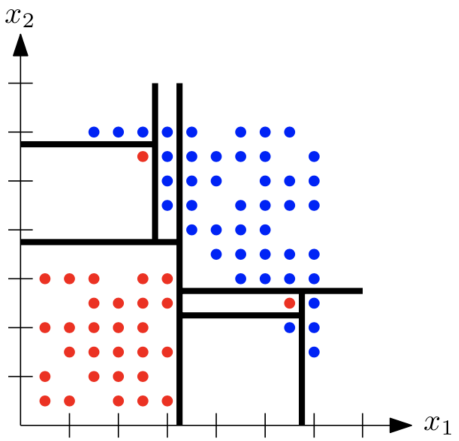
- **Hyperparameter:** specifics of learning algorithm $\mathcal{A}$
  - E.g. in DecisionTreeTrain, constrain to output tree of depth $\leq h$
  - Tuning hyperparameters often results in {over, under}-fitting

Hyperparameter tuning using validation set

- E.g. in decision tree training, how to choose tree depth $h \in \{1, \ldots, H\}$?

- For each hyperparameter $h \in \{1, \ldots, H\}$:
  - Train Tree_h using DecisionTreeTrain by constraining the tree depth to be h
- Choose one from $\mathrm{Tree}_1, \ldots, \mathrm{Tree}_H$



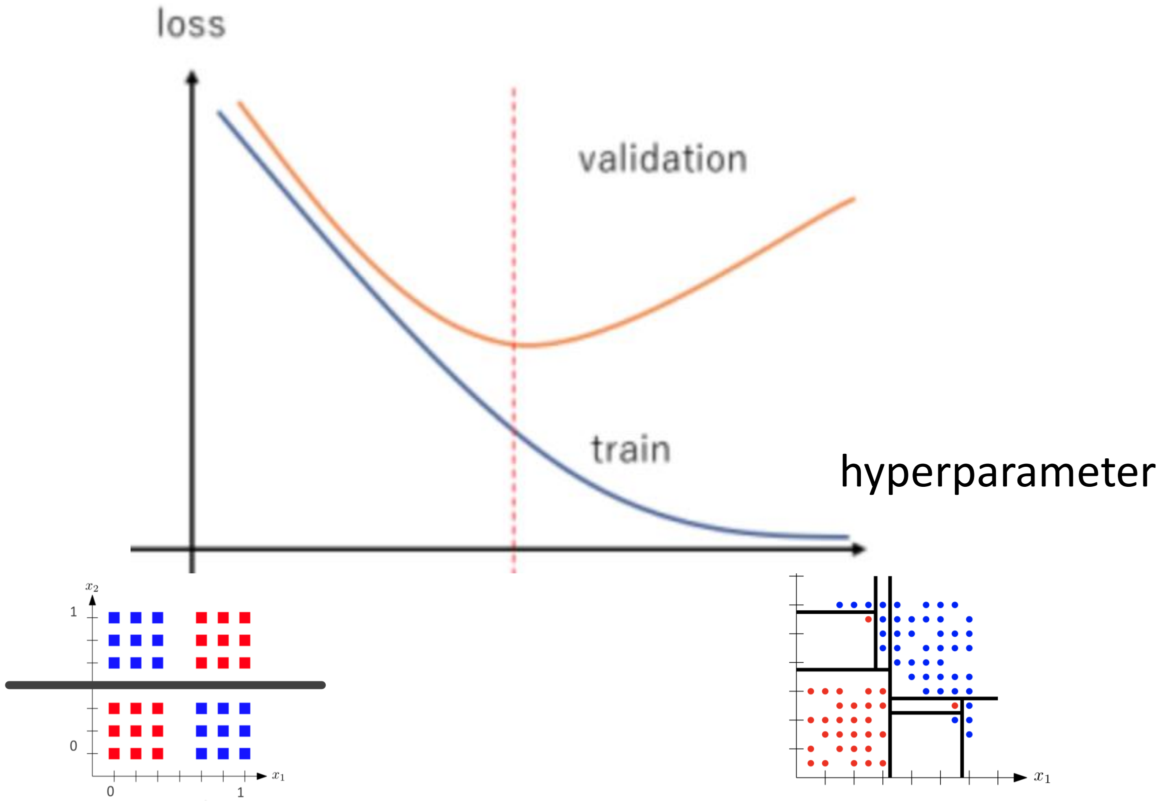


- Idea 1: choose Tree_h that minimizes training error
- Idea 2: choose Tree_h that minimizes test error
- Idea 3: further split training set to training set and validation set (development/hold-out set), (1) train Tree_h's using the (new) training set; (2) choose Tree_h that minimizes validation error

Training: 700 examples	Val:100 examples	Test: 200 examples

Hyperparameter tuning using validation set

- E.g. in decision tree training, how to choose tree depth $h \in \{1, \dots, H\}$?

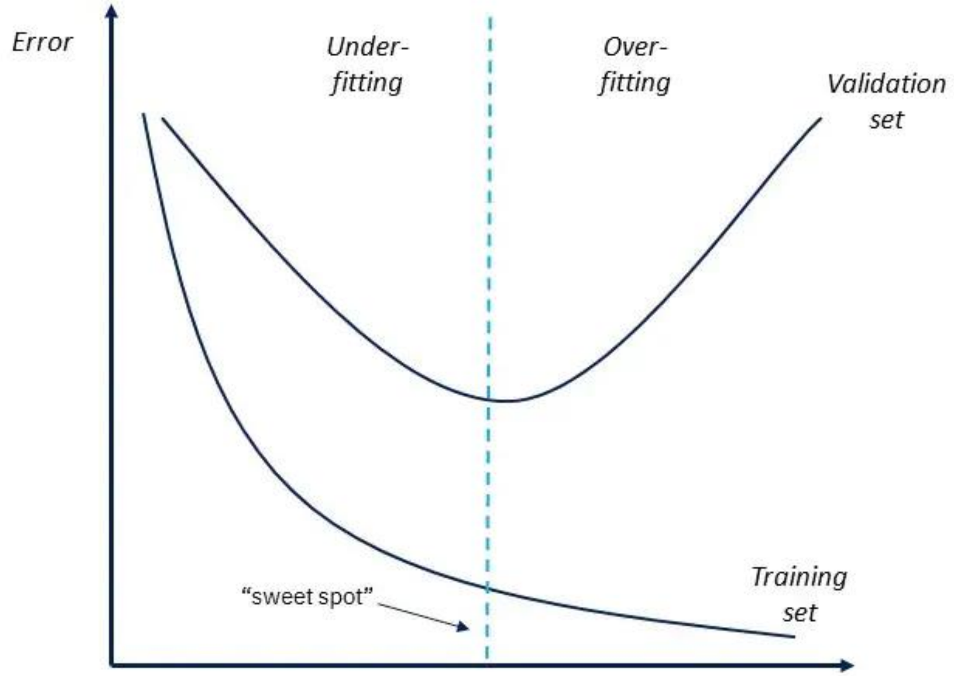


- Law of large numbers => Validation error closely approximates generalization error (& test error)

Overfitting vs Underfitting

Underfitting: performs poorly on *both* training and validation

Overfitting: performs well on training but not on validation



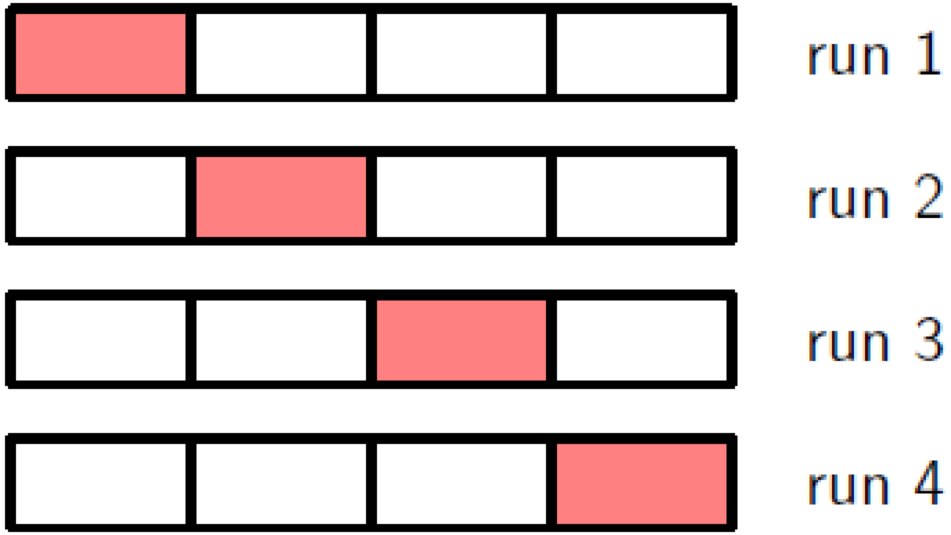
Source: ibm.com

hyperparameter

- Note: this U-shaped validation error curve may not always happen – "Benign overfitting" (Belkin et al, PNAS 2019)
- Nevertheless, choosing hyperparameters using validation error continues to be a good idea

Hyperparameter tuning: cross-validation

Main idea: improve data efficiency by splitting the training / validation data in multiple ways



N-fold Cross Validation: Partition training data into N "chunks" and for each run select one chunk to be validation data

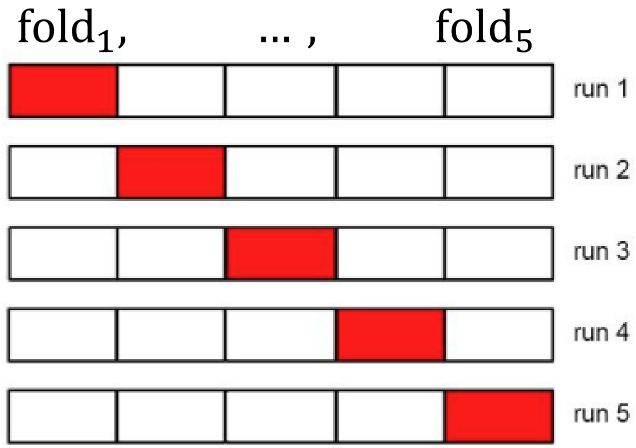
For each run, fit to training data (N-1 chunks) and measure accuracy on validation set. Average model error across all runs.

Source: Bishop, C. PRML

Cross-validation: formal description

- For hyperparameter $h \in \{1, \dots, H\}$
  - For $k \in \{1, \dots, K\}$
    - train f with $S \setminus \text{fold}_k$
    - measure error rate $e_{h,k}$ of f on fold_k
  - Compute the average error of the above: $E_h = \frac{1}{K} \sum_{k=1}^{K} e_{h,k}$
- Choose $\hat{h} = \arg\min_h E_h$
- Train $\hat{f}$ using S (all training examples) with hyperparameter $\hat{h}$

Training set S



- Typical K values: 5, 10
- Special case $K = |S|$: leave one out cross validation (LOOCV)

Miscellaneous concepts

Inductive bias

- What classification problem is class A vs. class B?
  - Birds vs. Non-birds
  - Flying animals vs. non-flying animals

class A

class B

- **<u>Inductive bias</u>**: in the absence of data that narrow down the target concept, what type of predictors are we likely to prefer?

- What is the inductive bias of learning shallow decision trees?

An example real-world machine learning pipeline

- Any step can go wrong
  - E.g. data collection, data representation
- Debugging suggestion: run *oracle experiments*
  - Assuming all lower-level tasks are perfectly done, is this step achieving what we want?
- General suggestions:
  - Build the stupidest thing that could possibly work
  - Decide whether / where to fix it

1	real world goal	increase revenue
2	real world mechanism	better ad display
3	learning problem	classify click-through
4	data collection	interaction w/ current system
5	collected data	query, ad, click
6	data representation	bow^2, $\pm$ click
7	select model family	decision trees, depth 20
8	select training data	subset from april'16
9	train model & hyperparams	final decision tree
10	predict on test data	subset from may'16
11	evaluate error	zero/one loss for $\pm$ click
12	deploy!	(hope we achieve our goal)

Next lecture (1/23)

- Geometric view of supervised learning; nearest neighbor methods

- Assigned reading: CIML Chap. 3 (Geometry and Nearest Neighbors)