Machine Learning: Supervised Methods
NOTES

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Contents

Abstract

These notes cover some of the key concepts in supervised learning. However it's not intended to be a comprehensive introduction into supervised methods. To get most out of the notes, one should have some base knowledge on machine learning and basic algebra.

Summary of Notation

The next list describes several symbols that will be later used within the body of the document.

log Natural logarithm (also commonly written as $\ln, \log_e$)

Part I

Theory

1 Introduction

1.1 Theoretical paradigms

Theoretical paradigms for machine learning **differ** mainly on what they assume about the process generating the data:

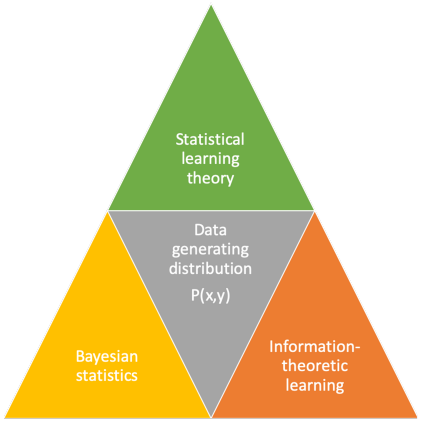

Figure 1: Paradigms for data generation distributions

- **Statistical learning theory (focus on this course):** assumes data is i.i.d from an unknown distribution P(x), does not estimate the distribution (directly)
- **Bayesian Statistics:** assumes prior information on P(x), estimates posterior probabilities
- **Information theoretic learning:** (e.g.Minimum Description Length principle, MDL): estimates distributions, but does not assume a prior on P(x)

1.2 Dimensions of a supervised learning algorithm

1. **Training sample:** $S = \{(x_i, y_i)\}_{i=1}^{m}$ the training examples $(x, y) \in X \times Y$ independently drawn from a identical distribution $(i.i.d)D$ defined on $X \times Y, X$ is a space of inputs, Y is the space of outputs.

2. **Model or hypothesis:** $h : X \to Y$ that we use to predict outputs given the inputs x.
3. **Loss function:** $L : Y \times Y \to \mathbb{R}, L(...) \geq 0, L(y, y')$ is the loss incurred when predicting y' when y is true.
4. **Optimization** procedure to find the hypothesis h that minimize the loss on the training sample.

1.3 Classification (Task 1/3)

Problem: partitioning the data into pre-defined classes by a *decision boundary* or *decision surface*.

Multi-class classification: more than two classes

- **Multi-label Classification:** An example can belong to multiple classes at the same time
- **Extreme classification:** Learning with thousands to hundreds of thousands of classes (Prof. Rohit Babbar @ Aalto)

1.3.1 Version space

Version space: the set of all consistent hypotheses of the hypothesis class

- **Consistent hypothesis:** if correctly classifies all training examples
- **In version space:**
  - **Most general hypothesis** G**:** cannot be expanded without including negative training examples
  - **Most specific hypothesis** S**:** cannot be made smaller without excluding positive training points

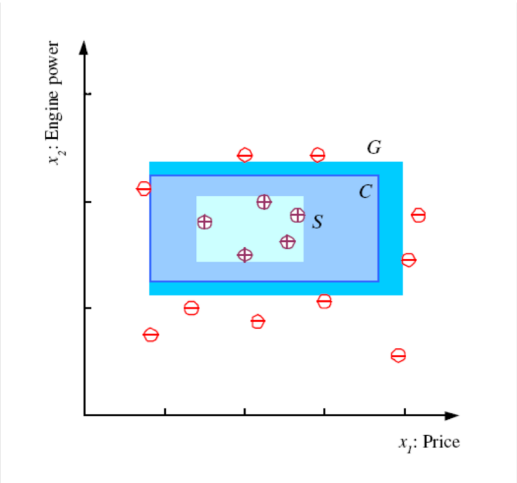

Figure 2: Illustration of a Version Space.

- Intuitively, the **"safest" hypothesis** to choose from the version space is the one that is furthers from the positive and negative training examples → maximum margin
  - Margin = minimum distance between the decision boundary and a training point

1.4 Regression (Task 2/3)

Problem: output variables which are numeric.

1.5 Ranking & preference learning (Task 3/3)

Problem: predict a ordered list of preferred objects.

Training data (typically): pairwise preferences.

- e.g. user x prefers movie y_i over movie y_j

Output: ranked list of elements.

1.6 Generalization

Aim: predict as well as possible the outputs of future examples, not only for training sample.

We would like to *minimize* the **generalization error**, or the **(true) risk**:

$$R(h) = E_{(x,y)\sim D}[L(h(x), y)] \tag{1}$$

Where:

D : Unknown distribution where from training and future examples are drawn from (i.i.d assumption)

What can we say about $R(h)$ based on training examples and the hypothesis class $\mathcal{H}$ alone? Two possibilities:

- Empirical evaluation by testing (Section 1.6.1)
- Statistical learning theory (Section 2)

1.6.1 Model evaluation by testing

What: estimate the model's ability to generalize on future data

How: approximating true risk by computing the empirical risk on a independent test sample:

$$R_{test}(h) = \sum_{(x_i,y_i)\in S_{test}}^{m} L(h(x_i), y_i)$$

- The expectation of $R_{test}(h)$ is the true risk $R(h)$

1.7 Hypothesis classes

There is a huge number of different **hypothesis classes** or **model families** in machine learning, **e.g:**

- **Linear models** such as logistic regression and perceptron
- **Neural networks:** compute non-linear input-output mappings through a network of simple computation units
- **Kernel methods:** implicitly compute non-linear mappings into high-dimensional feature spaces (e.g. SVMs)
- **Ensemble methods:** combine simpler models into powerful combined models (e.g. Random Forests)

Each have their different pros and cons in different dimensions (accuracy, efficiency, interpretability); No single best hypothesis class exists that would be superior to all others in all circumstances

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2 Statistical Learning Theory

What: Statistical learning theory focuses in analyzing the generalization ability of learning algorithms. It's the theoretical background on machine learning.

Goal: Generalization (Section 1.6)

2.1 Probably Approximately Correct (PAC) learning

What: The most studied *theoretical framework* for analyzing the generalization performance of machine learning algorithms. It formalizes the notion of generalization in machine learning. In practice, it's asking for bounding the generaliation error (ϵ) with high probability ($1-\delta$), with arbitrary level of error $\epsilon > 0$ and confidence $\delta > 0$.

Ingredients:

- **input space** X containing all possible **inputs** x
- set of possible **labels** Y (in binary classification $Y = \{0, 1\}$)
- **concept class** $\mathcal{C}$ contains **concepts** $C : X \to Y$ (to be learned), concept C gives a label $C(x)$ for each input x
  - underlying ground truth $\to$ to be learn in the ideal case
  - unknown in practice (or otherwise ML is not needed)
- Unknown (i.i.d) **probability distribution** D for the data
- **training sample** $S = (x_1, C(x_1)), ..., (x_m, C(x_m))$ drawn independently from D
- **hypothesis class** $\mathcal{H}$
  - in the **basic case** $\mathcal{H} = \mathcal{C}$ but this assumption can be relaxed

Goal: to learn a hypothesis with a low generalization error. For 0/1 loss:

$$R(h) = E_{x\sim D}[L_{0/1}(h(x), C(x))] = Pr_{x\sim D}(h(x) \neq C(x))$$

2.1.1 PAC learnability

What: Question, can we learn a concept class.

PAC-learnable concept class $\mathcal{C}$ if:

- if there exist an **algorithm** $\mathcal{A}$ that given a training sample S outputs a hypothesis $h_S \in \mathcal{H}$ that has generalization error satisfying

$$Pr(\underbrace{R(\overbrace{h_S}^{\text{chosen hypothesis from } \mathcal{H}}) \leq \epsilon}_{\text{"low generalization error" event}}) \geq \underbrace{1-\delta}_{\text{success rate}} \tag{2}$$

$P(GeneralizationError\ of\ h_S \leq GeneralizationError\ of\ interest) \geq Desired\ SuccessRate$
$P(selection\ hypothesis\ (from\ \mathcal{H})\ with\ GeneralizationError \leq \epsilon) \geq Desired\ SuccessRate$
$Probability\ of\ low\ GeneralizationError \geq Desired\ SuccessRate$

Where:

h_S**:** output hypothesis
S**:** training sample
$m = |S|$**:** sample size that grows polynomially in $1/\epsilon$, $1/\delta$
ϵ**:** generalization error of interest (arbitrary)
$1-\delta$**:** desired success rate / confidence (arbitrary)

Efficiently PAC-learnable concept class $\mathcal{C}$ if:

- **PAC-learnable**
- $\mathcal{A}$ runs in time polynomial in m, $1/\epsilon$, and $1/\delta$
  - We want the requirement for training data and running time **not to explode** when we make ϵ and δ stricter $\rightarrow$ requirement of polynomial growth

Interpretation:

- ϵ: sets the level of generalization error that is of interest to us
  - e.g. say we are satisfied with predicting incorrectly 10% of the new datapoints $\rightarrow \epsilon = 0.10$
- $1 - \delta$: sets a level of confidence that is of interest to us
  - e.g. say we are satisfied of the training algorithm to fail 5% of the time to provide a good hypothesis $\rightarrow \delta = 0.05$
- $\{R(h_S) \leq \epsilon\}$: The event "low generalization error"
  - considered as a *random variable* because we cannot know beforehand which hypothesis $h_S \in \mathcal{H}$ will be selected by the algorithm

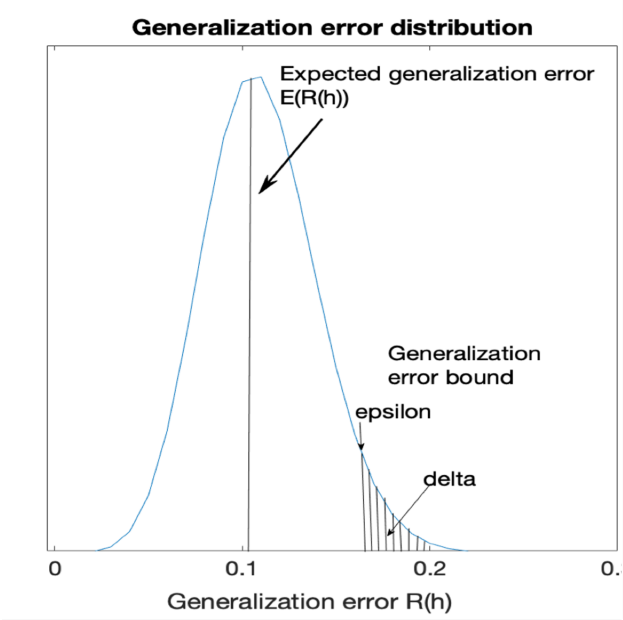


Figure 3: Generalization error distribution and error bound

Generalization error bound vs. expected test error:

- We bound the probability of being in the high error tail of the distribution (not the convergence to the mean or median generalization error) $\rightarrow$ thus **empirically estimated test errors** might be considerably lower than the bounds suggest.

2.2 Learning with finite hypothesis classes

What: Finite concept classes arise when:

- **Input variables** have finite domains or they are converted to such in preprocessing (e.g. discretizing real values)
- The representations of the hypotheses have finite size (e.g. the number of times a single variable can appear)

Finite hypothesis class - consistent case

- **Sample complexity bound** relying on the size of the hypothesis class (Mohri et al, 2018): $Pr(R(h_S) \leq \epsilon) \geq 1 - \delta$ if

$$m \geq \frac{1}{\epsilon}(log(|\mathcal{H}|) + log(\frac{1}{\delta}))$$

- An equivalent **generalization error bound**:

$$R(h) \leq \frac{1}{m}(log(|\mathcal{H}|) + log(\frac{1}{\delta}))$$

- **Holds for** any finite hypothesis class **assuming there is a** consistent hypothesis, one with zero empirical risk or close to it (relaxed).
- The more hypotheses there are in $\mathcal{H} \rightarrow$ the more training examples are needed

2.2.1 Example: Boolean conjunctions

What: Example of a finity hypothesis class.

Example hypothesis class: Boolean conjunctions

- Dealing with subclasses of Boolean formulae, expressions **binary input variables** (literals) combined with **logical operators** AND & NOT.

Example case: Aldo likes to do sport only when the weather is suitable

- **Training data:** Also has given examples of suitable and not suitable weather

	x^t						$r(x^t)$
t	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	1
2	Sunny	Warm	High	Strong	Warm	Same	1
3	Rainy	Cold	High	Strong	Warm	Change	0
4	Sunny	Warm	High	Strong	Cool	Change	1

Table: Aldo's observed sport experiences in different weather conditions.

- **Model:** Let us build a classifier (boolean formulae containing AND, and NOT, but not OR operators) for Aldo to decide whether to do sports today
  - e.g. if (Sky=Sunny) AND NOT (Wind=Strong) then (EnjoySport=1)
- **Number of hypotheses $|\mathcal{H}|$:**
  - **Each variable:** "AND", "AND NOT", or can be excluded from the rule $\rightarrow$ 3 possibilities
  - **Total number of hypotheses** is thus 3^d, where d is the number of variables $\rightarrow |\mathcal{H}| = 3^6 = 729$
- **Plotting the bound for Aldo's problem using boolean conjunctions:**
  - **Left plot:** generalization bound ϵ is shown for different values of delta δ, using d = 6 variables.

– **Right plot:** generalization bound ϵ is shown for increasing number of input variables d, using delta $\delta = 0.05$

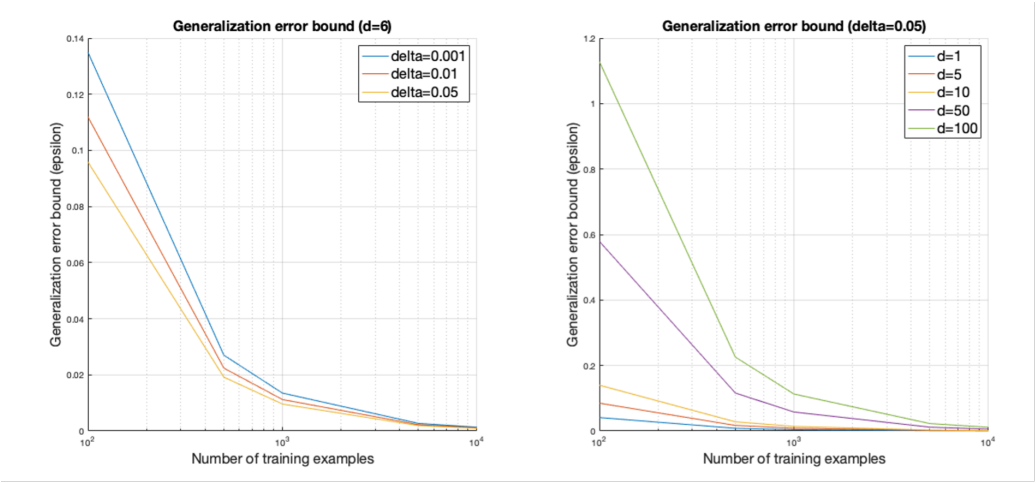


Figure 4: Boolean conjunctions: Generalization error bounds

- **Typical behaviour of ML learning algorithms is revealed:**
  - **increase of sample size decreases generalization error**
  - extra data gives **less and less additional benefit as the sample size grows** (law of diminishing returns)
  - requiring high level of confidence (small δ) for obtaining low error requires more data for the same level of error

2.3 Learning with infinite hypothesis classes

Most models used in practise rely on infinite hypothesis classes, e.g.

- $\mathcal{H}$ = hyperplanes in $\mathbb{R}^d$ (e.g. Support vector machines)
- $\mathcal{H}$ = neural networks with continuous input variables

2.3.1 Vapnik-Chervonenkis (VC) dimension

Purpose: Vapnik-Chervonenkis dimension lets us **study** learnability of infinite hypothesis classes **through** the concept of shattering

What: can be understood as measuring the capacity of a hypothesis class to adapt to different concepts

- $VCdim(\mathcal{H})$ = size of the **largest training set** that we can find a **consistent classifier for all labelings in** Y^m
- Intuitively:
  - low $VCdim \rightarrow$ easy to learn, low sample complexity
  - high $VCdim \rightarrow$ hard to learn, high sample complexity
  - infinite $VCdim \rightarrow$ cannot learn in PAC framework

How to show that $VCdim(\mathcal{H}) = d$ for a hypothesis class:

- We need to show two facts:
  1. There exists a set of inputs of size d that **can be shattered** by hypothesis in $\mathcal{H}$ (i.e. we can pick the set of inputs any way we like): $VCdim(\mathcal{H}) \geq d$
  2. There does not exist any set of inputs of size $d+1$ that **can be shattered** (i.e. need to show a general property): $VCdim(\mathcal{H}) < d+1$

Formally: (for binary labelings)

- Through **growth function**:

$$\sqcap_{\mathcal{H}}(m) = \max_{\{x_1,...,x_m\} \subset X} |\{(h(x_1),...,h(x_m)) : h \in \mathcal{H}\}|$$

  - The growth function gives the maximum number of unique labelings the hypothesis class $\mathcal{H}$ can provide for an arbitrary set of input points

– The maximum of the growth function is 2^m for a set of m examples

- **Vapnik-Chervonenkis dimension** is then

$$VCdim(\mathcal{H}) = \max_m\{m|\sqcap_{\mathcal{H}}(m) = 2^m\}$$

2.3.1.1 Shattering

What: underlying concept in VC dimension

Given: a set of points $S = x_1, ..., x_m$ and a fixed class of functions $\mathcal{H}$

$\mathcal{H}$ is said to shatter S if: for any possible partition of S into positive S_+ and negative subset S_- we can find a hypothesis for which $h(x) = 1$ if and only if $x \in S_+$

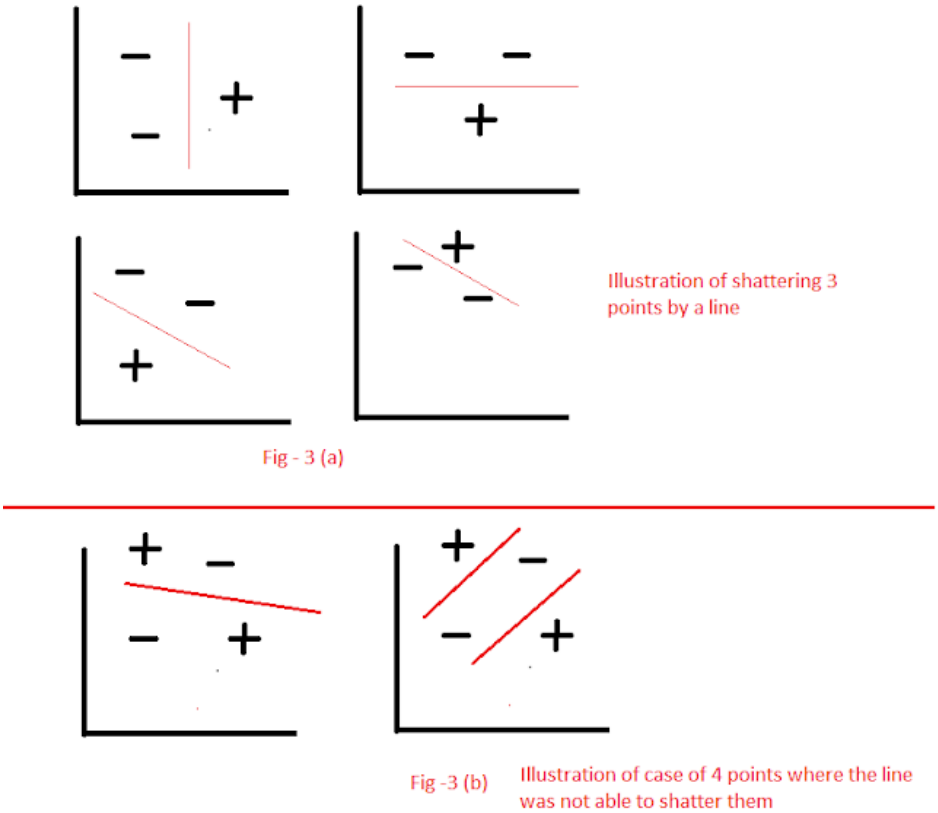


Figure 5: Illustration of shattering

2.3.1.2 Generalization bound with VC-dimension

What: Way of using VC-dimensions to analyze machine learning algorithms.

(Mohri, 2018) Let $\mathcal{H}$ be a family of functions taking values in $-1, +1$ with VC-dimension d . Then for any $\delta > 0$, with probability at least $1 - \delta$ the following holds for all $h \in \mathcal{H}$:

$$R(h) = \underbrace{\hat{R}(h)}_{\text{empirical risk}} + \sqrt{\frac{2\log(em/d)}{m/d}} + \sqrt{\frac{\log(1/\delta)}{2m}}$$

Where:

d**:** VC-dimension

m**:** amount of training data

e**:** Euler's number, $e \approx 2.71828$

δ**:** failure rate

- m/d shows that changing to a model with higher VC-dimension d makes the same amount of training samples m less effective. $\rightarrow$ the second term grows when VC-dimension grows.
  - For more complex $\mathcal{H}$ class, one needs more data m to guarantee similar kind of generalization.
- Manifestation of the **Occam's razor principle:** to justify an increase in the complexity, we need reciprocally more data

2.3.2 Rademacher complexity

What: Rademacher complexity defines complexity as the capacity of hypothesis class to fit random noise

Why: Rademacher complexity is a practical alternative to VC dimension, giving typically sharper bounds (but requires a lot of simulations to be run).

Experiment: how well does your hypothesis class fit noise?

- Consider a **set of training examples** $S_0 = \{(x_i, y_i)\}_{i=1}^m$
- **Generate** M **new datasets** $S_1, ..., S_M$ from S_0 by randomly drawing a new label $\sigma \in Y$ for each training example in S_0

$$S_k = \{(x_i, \sigma_{ik})\}_{i=1}^m$$

- Train a classifier h_k minimizing the empirical risk on training set S_k, record its empirical risk

$$\hat{R}(h_k) = \frac{1}{m} \sum_{i=1}^{m} 1_{h_k(x_i) \neq \sigma_{ik}}$$

- **Compute the average empirical risk over all datasets:**

$$\bar{\epsilon} = \frac{1}{M} \sum_{k=1}^{M} \hat{R}(h_k)$$

- **Observe the quantity:**

$$\hat{\mathcal{R}} = \frac{1}{2} - \bar{\epsilon}$$

  - When $(\hat{\mathcal{R}} = 0, \bar{\epsilon} = 0.5) \rightarrow$ predictions correspond to random coin flips (0.5 probability to predict either class)
  - When $(\hat{\mathcal{R}} = 0.5, \bar{\epsilon} = 0) \rightarrow$ all hypotheses $h_i, i = 1, ..., M$ have zero empirical error (perfect fit to noise, not good!)
  - **Ideally we want:**
    - to be able to **separate noise from signal**
      - Meaning large $\bar{\epsilon}$, so that the model is bad at classifying random noise. $\rightarrow$ low complexity $\hat{\mathcal{R}}$.
    - to have **low empirical error on real data** - otherwise impossible to obtain low generalization error

Rademacher complexity:

- For binary classification with labels $Y = \{-1, +1\}$ **empirical Rademacher complexity** can be defined as

$$\hat{\mathcal{R}}_S(\mathcal{H}) = \frac{1}{2} E_\sigma \underbrace{(\sup_{h \in \mathcal{H}} \frac{1}{m} \sum_{t=1}^{m} \overbrace{\sigma^i}^{\text{random true label}} \overbrace{h(x_i)}^{\text{predicted random label}})}_{\text{hypothesis with highest correlation with random label}}$$

Where:

$\sigma_i \in \{-1, +1\}$**:** are Rademacher random variables, drawn independently from uniform distribution (i.e. $Pr\{\sigma = 1\} = 0.5$)

- We can also rewrite $\hat{\mathcal{R}}_S$ **in terms of empirical error**

$$\hat{\mathcal{R}}_S = \frac{1}{2} - E_\sigma \inf_{h \in \mathcal{H}} \hat{\epsilon}(h)$$

  - Now we have Rademacher complexity in terms of expected minimum error of classifying randomly labeled data

2.3.2.1 Generalization bound with Rademacher complexity

(Mohri et al. 2018): For any $\delta > 0$, with probability at least $1 - \delta$ over a sample drawn from an unknown distribution D, for any $h \in \mathcal{H}$ we have:

$$R(h) \leq \underbrace{\hat{R}_S(h)}_{\text{empirical risk}} + \underbrace{\hat{\mathcal{R}}_S(\mathcal{H})}_{\text{empirical Rademacher complexity}} + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

2.3.3 Vapnik-Chervonenkis dimension VS. Rademacher complexity

Note the differences between Rademacher complexity and VC dimension

- Dependency on training data

- **VC dimension:** independent → measures the worst-case where the data is generated in a bad way for the learner
- **Rademacher complexity:** depends on the training sample thus is dependent on the data generating distribution

- Focus
  - **VC dimension:** extreme case of realizing all labelings of the data
  - **Rademacher complexity:** measures smoothly the ability to realize random labelings

Example: Rademacher and VC bounds on a real dataset

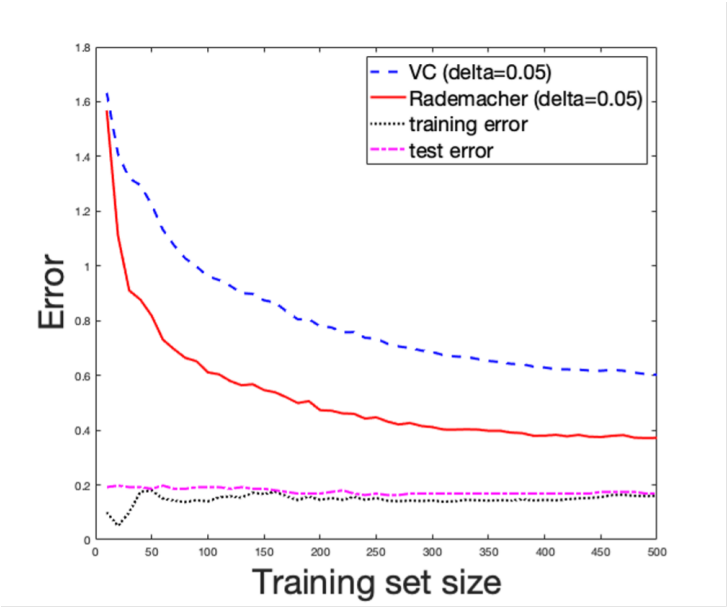


Figure 6: Rademacher and VC bounds on a real dataset

- Rademacher bound is sharper than the VC bound
- VC bound is not yet informative with 500 examples (> 0.5) using ($\delta = 0.05$)
- The gap between the mean of the error distribution ($\approx$ test error) and the 0.05 probability tail (VC and Rademacher bounds) is evident (and expected)

3 Model selection

Key principle: Model selection in machine learning can be seen to implement Occam's razor:

- **Occam's razor, (principle of parsimony)** is the *problem-solving principle* that "entities should not be multiplied beyond necessity".
- **Simply:** If there are several equally correct explanations for some phenomenon, the simplest explanation is the most preferred one.

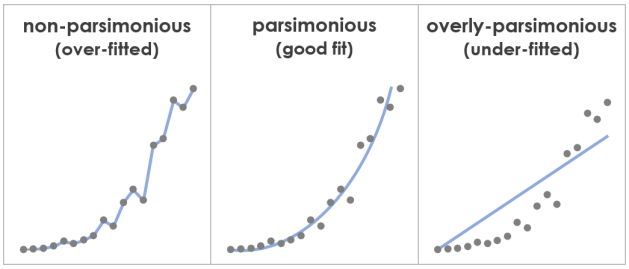


Figure 7: Illustration of parsimony in the context of ML models

- **In model selection:** captures the trade-off between generalization error (bias & variance) and model complexity.

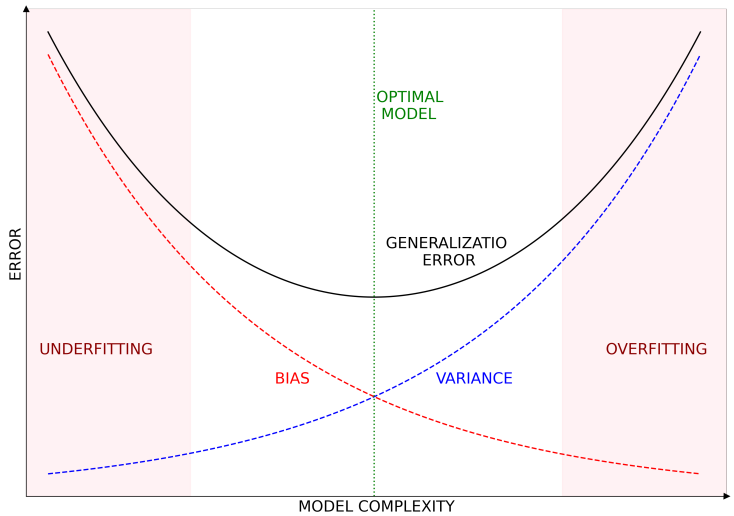


Figure 8: Illustration of parsimony in the context of ML models

Scenario – what we assume from the data:

- **So far- DETERMINISTIC SCENARIO:** The analysis so far assumed that the labels are deterministic functions of the input
- **Now- STOCHASTIC SCENARIO:** Relaxes this assumption by assuming the output is a probabilistic function of the input
  - Inputs X and outputs Y are generated by a joint probability distribution D or $X \times Y$
  - In the stochastic scenario, there **may not always exist a target concept** f that has zero generalization error $R(f) = 0$

Sources of stochasticity: stochastic dependency between input and output can arise from various sources

- Imprecision in recording the input data (e.g. measurement error), shifting our examples
- Errors in the labeling of the training data (e.g. human annotation errors), flipping the labels some examples
- There may be additional variables that affect the labels that are not part of our input data

All of these sources of stochasticity could be characterized as adding **noise** (or **hiding signal**)

NOISE (All sources of stochasticity) and Complexity:

- **Typical effect:** make the decision boundary more complex (e.g. a spline curve instead of a hyperplane). But this may not give a better generalization error, **if** we end up merely re-classifying points corrupted by noise.
- In practice, we need to **balance** the complexity of the hypothesis and the empirical error carefully
  - A **too simple model** does not allow optimal empirical error to obtained, this is called underfitting

– A **too complex model** may obtain zero empirical error, but have worse than optimal generalization error, this is called overfitting

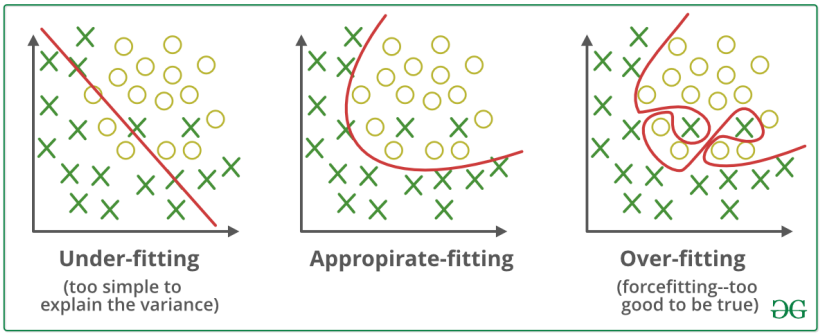


Figure 9: Illustration of under- and overfitting

Controlling complexity (2 general approaches):

1. **Hypothesis Class selection:** e.g. the maximum degree of polynomial to fit the regression model
2. **Regularization:** penalizing the use of too many parameters

Measuring complexity

- We have already looked at some measures:
  - **Number of distinct hypotheses $|\mathcal{H}|$:** works for finite $\mathcal{H}$
  - **Vapnik-Chervonenkis dimension (VCdim) (Section 2.3.1):** the maximum number of examples that can be classified in all possible ways by choosing different hypotheses $h \in \mathcal{H}$
  - **Rademacher complexity (Section 2.3.2):** measures the capability to classify after randomizing the labels
- Lots of other complexity measures and model selection methods exist (not in the scope here)

3.1 Bayes error

Bayes error is the minimum achievable error (non-zero), given a distribution D over $X \times Y$ (*stochastic scenario*), by measurable functions $h : X \to Y$

$$R^* = \inf_{\{h|h\ measurable\}} R(h)$$

- Note that we cannot actually compute $R^* \to$ serves us as a theoretical measure of best possible performance

Bayes classifier is a hypothesis with $R(h) = R^*$

$$h_{Bayes}(x) = \arg\max_{y \in \{0,1\}} Pr(y|x)$$

- The average error made by the Bayes classifer at $x \in X$ is called the **noise**:
$$noise(x) = \min(Pr(1|x), Pr(0|x))$$
  - Its expectation $E(noise(x)) = R^*$ is the Bayes error
- Similarly to the Bayer error, Bayes classifier is a theoretical tool of best possible classifier, not something we can compute in practice

3.2 Decomposing the error of a hypothesis

The **excess error** of a hypothesis h compared to the Bayes error R^* can be decomposed as:

$$R(h) - R^* = \underbrace{\underbrace{\epsilon_{estimation}}_{\text{variance}} + \underbrace{\epsilon_{approximation}}_{\text{bias}}}_{\text{bias-variance decomposition}}$$

- $\epsilon_{estimation}(variance) = R(h) - R(h^*)$ is the excess generalization error h has over the optimal hypothesis $h^* = \arg\min_{h' \in \mathcal{H}} R(h')$ in the hypothesis class $\mathcal{H}$
- $\epsilon_{approximation}(bias) = R(h^*) - R^* =$ is the approximation error due to selecting the hypothesis class $\mathcal{H}$ instead of the best possible hypothesis class (which is generally unknown to us)

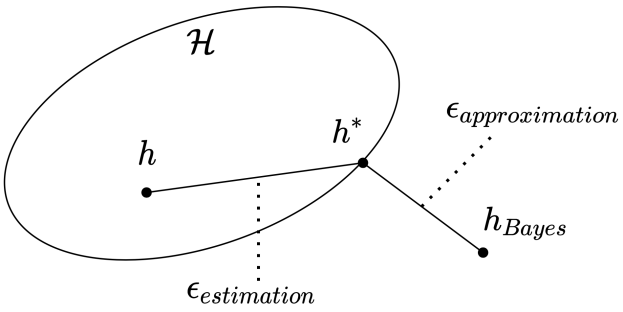


Figure 10: Illustration depicting the concepts

- h_{Bayes} is the Bayes classifier, with $R(h_{Bayes}) = R^*$
- $h^* = \inf_{h \in \mathcal{H}} R(h)$ is the hypothesis with the lowest generalization error in the hypothesis class $\mathcal{H}$
- $R(h)$ has both non-zero estimation error $R(h) - R(h^*)$ and approximation error $R(h^*) - R(h_{Bayes})$
- **Challenge for model selection:** We can bound the estimation error by generalization bounds but we cannot do the same for the approximation error as R^* remains unknown to us.

3.3 Strategies for Model Selection

Initially choose a very complex hypothesis class with zero or very low empirical risk $\mathcal{H}$

Assume the class can be decomposed into a union of increasingly complex hypothesis classes $\mathcal{H} = \bigcup_{\gamma \in \Gamma} \mathcal{H}_\gamma$

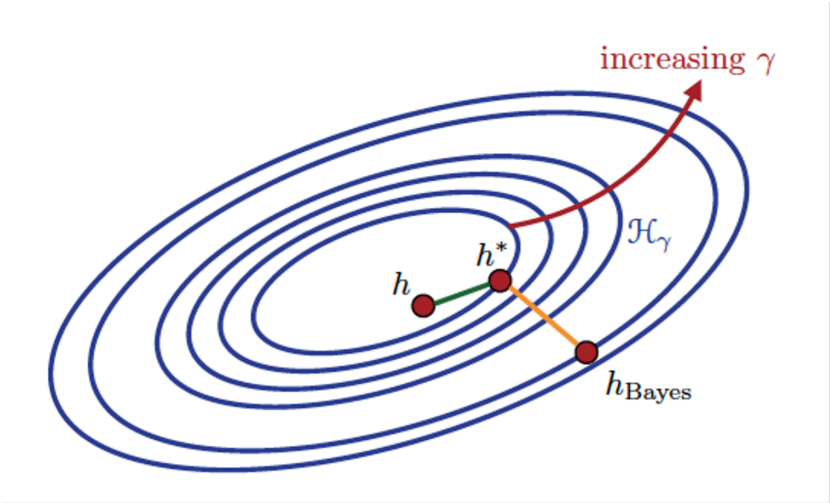


Figure 11: Illustration of hypothesis classes $\mathcal{H}$ being decomposed into a union of increasingly complex hypothesis classes

- The complexity increases by parameter γ e.g.
  - γ = degree of a polynomial function
  - γ = size of a neural network
  - γ = norm of weights of a linear regression model

Strategy:

- **The model selection problem then entails** choosing a parameter value λ^* that gives the best generalization performance

Trade-Off: increasing the complexity of the hypothesis class

- (+) complexity → (−) approximation error (as the class is more likely to contain a hypothesis with error close to the Bayes error)
- (+) complexity → (+) estimation error (as finding the good hypothesis becomes more hard and the generalization bounds become looser (due to increasing log $\mathcal{H}_\gamma$ or the VC dimension))

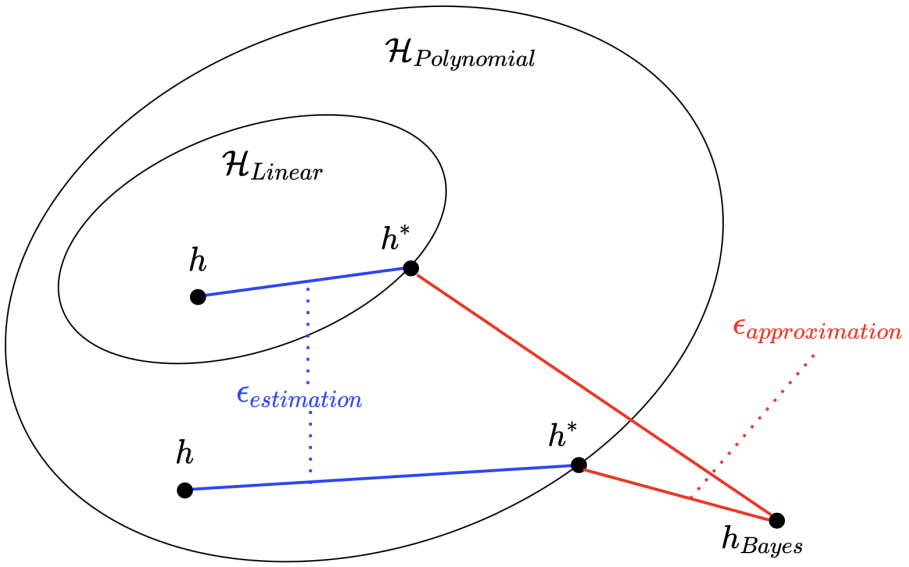


Figure 12: Example case of two hypothesis h from decomposed hypothesis classes $\mathcal{H}$, and their relation to h_{Bayes}

To minimize the generalization error over all hypothesis classes, we should find a balance between the two terms

3.3.1 Structural Risk Minimization (SRM)

What: An *inductive principle* of use in ML.

- **Assumes** a countable union of hypothesis classes $\mathcal{H} = \bigcup_{k \geq 1} \mathcal{H}_k$, indexed by complexity parameter k
- **Model selection task:** Select the optimal index k^* and the hypothesis $h \in \mathcal{H}_{k^*}$ that gives the best generalization bound

Why: It aims to minimize the excess risk $R(h) - R(h_{Bayes})$.

How: By bounding $R(h)$.

- **Generalization bound for SRM (Mohri et al. 2018) in PAC-framework:** for any $\delta > 0$ with probability at least $1 - \delta$ over the

draw of a sample S of size m, we have for all $k \geq 1$ and $h \in \mathcal{H}_k$

$$R(h) \leq \underbrace{\hat{R}_S(h)}_{\substack{\text{empirical error} \\ \text{on training set}}} + \underbrace{R_m(\mathcal{H}_k(h))}_{\substack{\text{Rademacher complexity of} \\ \text{least complex hypothesis class} \\ (\min k \text{ for } \mathcal{H}) \text{ where } h \text{ belongs}}} + \underbrace{\sqrt{\frac{\log k}{m}}}_{\substack{\text{penalty for not} \\ \text{knowing the correct } \mathcal{H} \\ (\mathcal{H} \text{ selection})}} + \sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

– See resemblance to 2.3.2.1.

SRM model selection algorithm: Given a training sample S, picks the index k and $h_S^{SRM} \in \mathcal{H}_k$ that minimizes

$$h_S^{SRM} = \underset{k \geq 1, h \in \mathcal{H}_k}{\arg\min}\, \hat{R}_S(h) + R_m(h_k) + \sqrt{\frac{\log k}{m}}$$

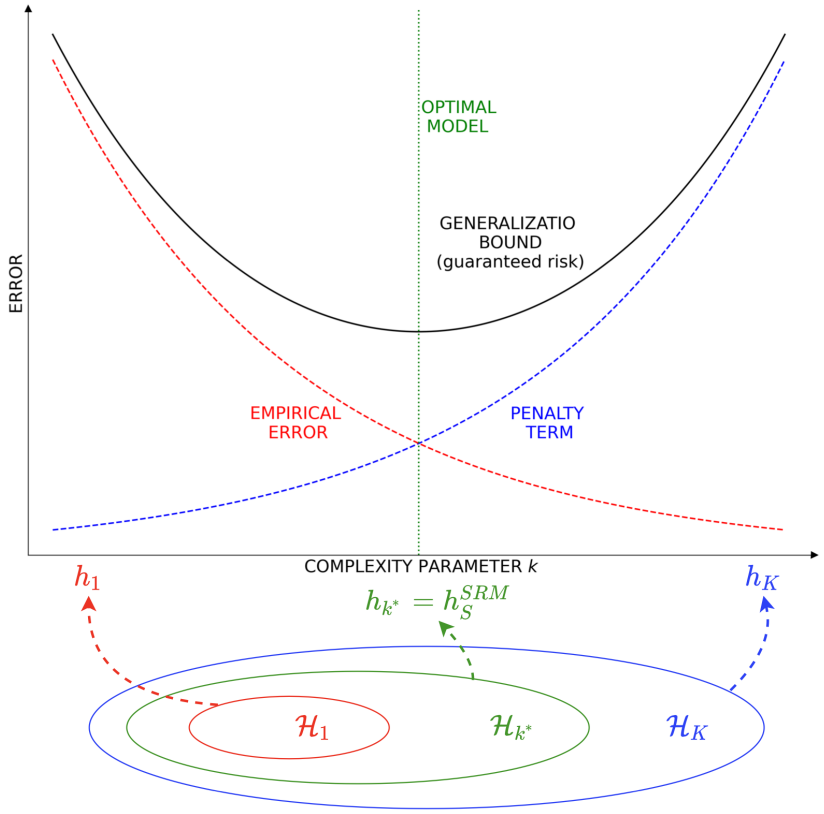


Figure 13: Illustration of Structural Risk Minimization (SRM) with Rademacher complexity

- **Note** that this may be a computationally difficult task:
  - Requires finding the hypothesis that minimizes training error for each hypothesis class separately
  - Obtaining the empirical Rademacher complexity generally requires simulation with multiple datasets with randomized labels for each hypothesis class

Pros & Cons of SRM:

\+ benefits from strong learning guarantees

− restrictive assumption of a countable decomposition of the hypothesis class

− large computational price, especially when a large number of hypothesis classes $\mathcal{H}_k$ has to be processed

3.3.2 Regularization-based algorithms

What: An alternative model selection approach to SRM.

- **Assumes** a very complex family $\mathcal{H} = \bigcup_{\gamma \geq 0} \mathcal{H}_\gamma$ of uncountable union of nested hypothesis classes $\mathcal{H}_\gamma$

How:

This extension to the SRM method would then ask to minimize:

$$= \underset{\gamma \geq 0, h \in \mathcal{H}_\gamma}{\arg\min} \hat{R}_S(h) + R_m(h_\gamma) + \sqrt{\frac{\log \gamma}{m}}$$

- This problem seems to require evaluating the Rademacher complexity of an uncountably infinite number of hypothesis classes $\mathcal{H}_\gamma \rightarrow$ Need efficient algorithms to do this

However this kind of model selection is efficient for the class of **linear functions** $x \rightarrow w^T x$

- The classes as parametrized by the norm $||w||$ of the weight vector bounded by γ:

$$\mathcal{H}_\gamma = \{x \to w^T x : ||w|| \leq \gamma\}$$

  - The norm $||w||$ is typically eiteher:
    - L^2 **norm (Also called Euclidean norm or 2-norm):**
      - used e.g. in support vector machines and ridge regression

$$||w||_2 = \sqrt{\sum_{j=1}^{n} w_j^2}$$

    - L^1 **norm (Also called Manhattan norm or 1-norm):**
      - used e.g. in LASSO regression

$$||w||_1 = \sum_{j=1}^{n} |w_j|$$

Computational shortcut: for L^2-norm: the empirical Rademacher complexity of this class can be bounded analytically!

- Let $S \subset \{x \mid \ ||x|| \leq r\}$ be a sample of size m and let $\mathcal{H}_\gamma = \{x \to w^T x : ||w||_2 \leq \gamma\}$. Then

$$\hat{R}_S(\mathcal{H}_\gamma) \leq \sqrt{\frac{r^2\gamma^2}{m}} = \frac{r\gamma}{\sqrt{m}}$$

Where:

r : upped bound for length of the input vector $||x||$

γ : upped bound for length of the weight vector $||w||_2$

  - Thus the **Rademacher complexity** depends linearly on the upper bound γ norm of the weight vector, as r and m are constant for any fixed training set
  - So we can use $||w||$ as a efficiently computable upper bound of $hat R_S(\mathcal{H}_\gamma)$

Regularized learning problem: minimize

$$\arg\min_{h \in \mathcal{H}} \hat{R}_S(h) + \lambda \Omega(h)$$

Where:

$\hat{R}_S(h)$: empirical error

$\Omega(h)$: regularization term which increases when the complexity of the hypothesis class increases

λ : regularization parameter, which is usually set by cross-validation

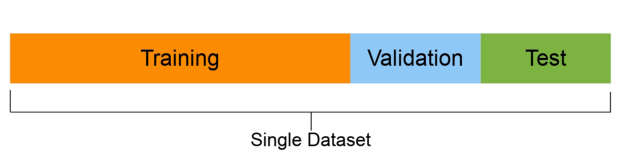
3.3.3 Model selection using a validation set

What: Using the given dataset for *empirical model selection*.

When: *If* the algorihm has input parameters (hyperparameters) that define/affect the model complexity.

How:

1. **Split** the data into training, validation and test sets



2. Use **grid search** to find the hyperparameters combination that gives the best performance on the validation set
   - In its **basic form** it goes through all combinations of parameter values, given a set of candidate values for each parameter
     - **With many hyperparameters** the search becomes computationally hard due to exponentially exploding search space
3. **Retrain a final model** using the *optimal parameter combination*, use both the training and validation data for training
4. **Evaluate the performance** of the final model on the test set

Sets:

- **Training set:** used to fit (optimize) the parameters (weights) of the model.
- **Validation set:** used to avoid overfitting. It provides an unbiased evaluation of a model fit on the training data set while tuning the model's hyperparameters.
- **Test set:** used to obtain reliable performance estimate.

Deciding on set sizes:

- The **larger the training set**, the better the generalization error will be (e.g. by PAC theory)
- The **larger the validation set**, the less variance there is in the test error estimate.
- When the **dataset is small** generally the **training set** is taken to be as large as possible, typically 90% or more of the total
- When the **dataset is large**, **training set** size is often taken as big as the computational resources allow

Stratification: is a process that tries to ensure similar class distributions across the different sets.

- **Motivation:** Class distributions of the training and validation sets should be as similar to each another as possible, otherwise there will be extra unwanted variance
- **Simple approach:** divide all classes separately into the training and validation sets and the merge the class-specific training sets into global training set and class-specific validation sets into a global validation set.

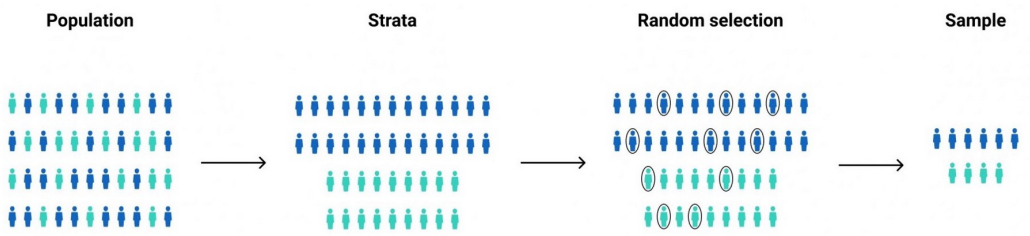


Figure 14: Illustration of stratified sampling

3.3.4 Cross-validation

Why: One split of data into training, validation and test sets may not be enough, due to randomness:

- The training and validation sets might be small and contain noise or outliers
- There might be some randomness in the training procedure (e.g. initialization)

How: Fighting the randomnes by averaging the evaluation measure over multiple (training, validation) splits

- → The **best hyperparameter values** are chosen as those that have the best average performance over the n validation sets.

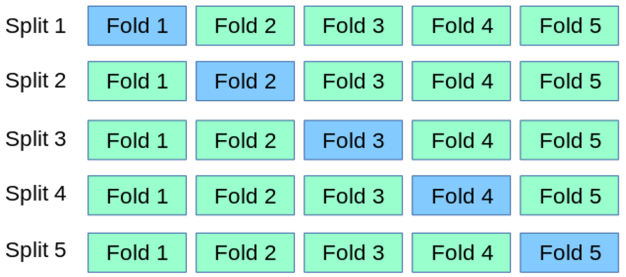
Various cross-validation schemes can be used to tackle the variance of the performance estimates.

n-Fold Cross-Validation

1. First **set a side** a separate test set
2. Then **split the remaining data randomly** into n equal-sized parts (or folds)

- $n = 5$ or $n = 10$ are typical numbers used in practice

3. Keep **one of the** n **folds** as the validation set (light blue in the Figure) and combine the **remaining** $n - 1$ **folds** to form the training set for the split



Leave-one-out Cross-Validation (LOO)

- **How:** given a dataset of m examples, only one example is left out as the validation set and training uses the $m - 1$ examples.
- **Has good theoretical properties:** This gives an unbiased estimate of the average generalization error over samples of size $m - 1$ (Mohri, et al. 2018, Theorem 5.4.)
- However, **if** m **is large**, it is comptationally demanding to compute

Nested cross-validation

- **Motivation:** only using a **single test set** may result in unwanted variation → Nested cross-validation solves this problem by using two cross-validation loops
- **Process:**
  1. The dataset is initially divided into n outer folds
  2. **Outer loop** uses **1 fold** at a time as a **test set**,
  3. The **remaining folds** of the data is used in the **inner fold**
     - **Inner loop** splits the remaining exampls into k folds, 1 fold for validation, and $k - 1$ for training

4. The average performance over the n test sets is computed as the **final performance estimate**

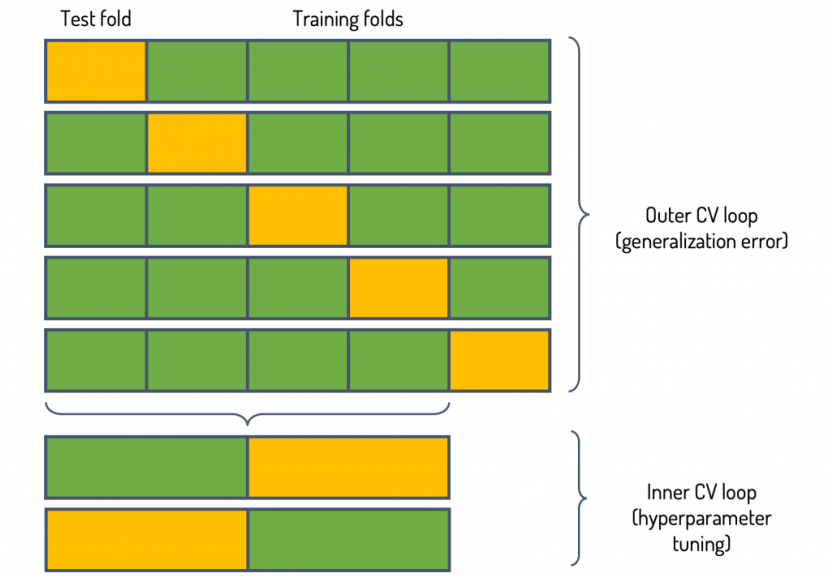


Figure 15: Illustration of 5×2 nested cross-validation