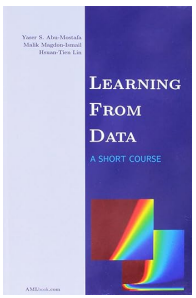
UNIVERSITY OF MARYLAND

MSML610: Advanced Machine Learning

Machine Learning Theories



Instructor: Dr. GP Saggese - gsaggese@umd.edu

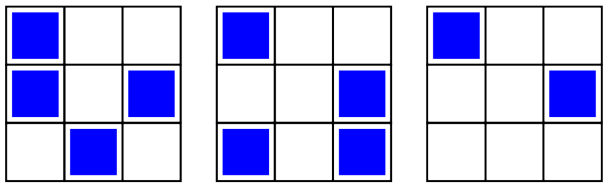
References:

- Abu-Mostafa et al.: *"Learning From Data"* (2012)

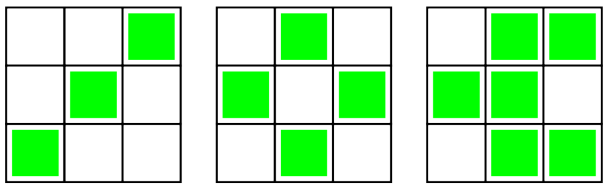
- ***Is Machine Learning Even Possible?***
- Growth Function
- The VC Dimension
- Overfitting
- Bias Variance Analysis
- Learning Curves
- Learn-Validation Approach

A Simple Visual ML Experiment (1/2)

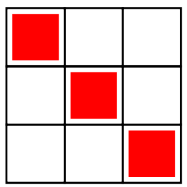
- Consider the supervised classification problem
- **Input**
  - A 9 bit vector represented as a 3x3 array
- **Training set**
  - The blue row $\underline{x}_1, \underline{x}_2, \underline{x}_3$ for $f(\underline{x}) = -1$
  - The green row $\underline{x}_4, \underline{x}_5, \underline{x}_6$ for $f(\underline{x}) = +1$
- **Test set**
  - For the red pattern $\underline{x}_0$, is $f(\underline{x}_0) = -1$ or $+1$?



$f = -1$



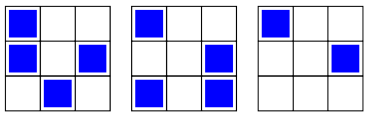
$f = +1$

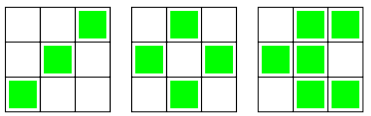


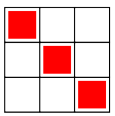
$f = ?$

A Simple Visual ML Experiment (2/2)

- **Model 1**
  - $f(\underline{\boldsymbol{x}}) = +1$ when $\underline{\boldsymbol{x}}$ has an axis of symmetry
  - $f(\underline{\boldsymbol{x}}) = -1$ when $\underline{\boldsymbol{x}}$ is not symmetric
  - The test set is symmetrical $\implies f(\underline{\boldsymbol{x}}_0) = +1$
- **Model 2**
  - $f(\underline{\boldsymbol{x}}) = +1$ when the top left square $\underline{\boldsymbol{x}}$ is empty
  - $f(\underline{\boldsymbol{x}}) = -1$ when the top left square $\underline{\boldsymbol{x}}$ is full
  - The test set has top left square full $\implies f(\underline{\boldsymbol{x}}_0) = -1$
- Many functions fit the 6 training examples
  - Some have a value of -1 on the test point, others $+1$
  - Which one is it?
- How can a limited data set reveal enough information to define the entire target function?
  - **Is machine learning possible?**





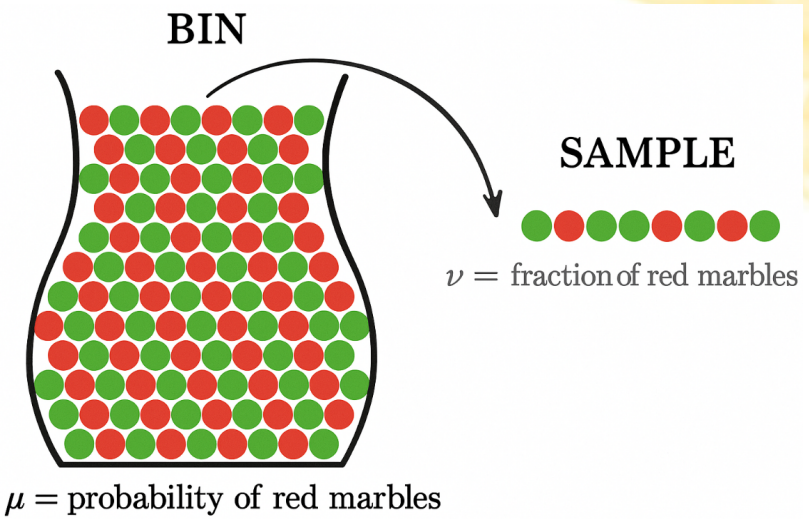


Is Machine Learning Possible?

- The function can assume **any value outside data**
  - E.g., with summer temperature data, the function could assume a different value for winter
- **How to learn an unknown function?**
  - Estimating at unseen points seems impossible in general
  - Requires assumptions or models about behavior
- Difference between:
  - **Possible**
    - No knowledge of the unknown function
    - E.g., could be linear, quadratic, or sine wave outside known data
  - **Probable**
    - Some knowledge of the unknown function from domain knowledge or historical data patterns
    - E.g., if historical weather data forms a sinusoidal pattern, unknown points likely follow that pattern

Supervised Learning: Bin Analogy (1/2)

- Consider a bin with red and green marbles
  - We want to estimate $\Pr(\text{pick a red marble}) = \mu$ where the value of μ is unknown
  - We pick N marbles independently with replacement
  - The fraction of red marbles is ν



- Does ν say anything about μ?
  - **"No"**
    - In strict terms, we don't know anything about the marbles we didn't pick
    - The sample can be mostly green, while the bin is mostly red
    - This is *possible*, but *not probable*
  - **"Yes"**
    - Under certain conditions, the sample frequency is close to the real frequency
- **Possible vs probable**
  - It is **possible** that we don't know anything about the marbles in the bin
  - It is **probable** that we know something
  - Hoeffding inequality makes this intuition formal

Hoeffding Inequality

- Consider a Bernoulli random variable X with probability of success μ
- Estimate the mean μ using N samples with $\nu = \frac{1}{N}\sum_i X_i$
- The **probably approximately correct** (PAC) statement holds:

$$\Pr(|\nu - \mu| > \varepsilon) \leq \frac{2}{e^{-2\varepsilon^2 N}}$$

- **Remarks:**
  - Valid for all N and ε, not an asymptotic result
  - Holds only if you sample ν and μ at random and in the same way
  - If N increases, it is exponentially small that ν will deviate from μ by more than ε
  - The bound does not depend on μ
  - Trade-off between N, ε, and the bound:
    - Smaller ε requires larger N for the same probability bound
    - Since $\nu \in [\mu - \varepsilon, \mu + \varepsilon]$, you want small ε with a large probability
  - It is a statement about ν and not μ although you use it to state something about ν (like for a confidence interval)

Supervised Learning: Bin Analogy (2/2)

- Let's connect the bin analogy, Hoeffding inequality, and feasibility of machine learning
  - You know $f(\underline{\boldsymbol{x}})$ at points $\underline{\boldsymbol{x}} \in \mathcal{X}$
  - You choose an hypothesis $h : \mathcal{X} \to \mathcal{Y} = \{0, 1\}$
  - Each point $\underline{\boldsymbol{x}} \in \mathcal{X}$ is a marble
  - You color red if the hypothesis is correct $h(\underline{\boldsymbol{x}}) = f(\underline{\boldsymbol{x}})$, green otherwise
  - The in-sample error $E_{in}(h)$ corresponds to ν
  - The marbles of unknown color corresponds to $E_{out}(h) = \mu$
  - $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_n$ are picked randomly and independently from a distribution over $\mathcal{X}$ which is the same as for E_{out}
- Hoeffding inequality holds and bounds the error going from in-sample to out-of-sample

$$\Pr(|E_{in} - E_{out}| > \varepsilon) \leq c$$

  - Generalization over unknown points (i.e., marbles) is possible
  - **Machine learning is possible!**

Validation vs Learning: Bin Analogy

- You have learned that for a given h, in-sample performance $E_{in}(h) = \nu$ needs to be close to out-of-sample performance $E_{out}(h) = \mu$
  - This is the **validation setup**, after you have already learned a model
- In a **learning setup** you have h to choose from M hypotheses
  - You need a bound on the out-of-sample performance of the chosen hypothesis $h \in \mathcal{H}$, regardless of which hypothesis you choose
  - You need a Hoeffding counterpart for the case of choosing from multiple hypotheses

$$\begin{aligned}
\forall g \in \mathcal{H} = \{h_1, ..., h_M\} \ \Pr(|E_{in}(g) - E_{out}(g)| > \varepsilon) \\
&\leq \Pr(\bigcup_{i=1}^{M}(|E_{in}(h_i) - E_{out}(h_i)| > \varepsilon)) \\
&\leq \sum_{i=1}^{M} \Pr(|E_{in}(h_i) - E_{out}(h_i)| > \varepsilon) && \text{(by the union bound)} \\
&\leq 2M \exp(-2\varepsilon^2 N) && \text{(by Hoeffding)}
\end{aligned}$$

Problem: the bound is weak

Validation vs Learning: Coin Analogy

- In a **validation set-up**, you have a coin and want to determine if it is fair
- Assume the coin is unbiased: $\mu = 0.5$
- Toss the coin 10 times
- How likely is that you get 10 heads (i.e., the coin looks biased $\nu = 0$)?

$$\Pr(\text{coin shows } \nu = 0) = 1/2^{10} = 1/1024 \approx 0.1\%$$

- **Conclusion**: the probability that the out-of-sample performance ($\nu = 0.0$) is completely different from the in-sample perf ($\mu = 0.5$) is very low

Validation vs Learning: Coin Analogy

- In a **learning set-up**, you have many coins and you need to choose one and determine if it's fair
- If you have 1000 fair coins, how likely is it that at least one appears totally biased using 10 experiments?
  - I.e., out-of-sample performance is completely different from in-sample performance

$$\begin{aligned}\Pr(\text{at least one coin has } \nu = 0) &= 1 - \Pr(\text{all coins have } \nu \neq 0) \\ &= 1 - (\Pr(\text{a coin has } \nu \neq 0))^{10} \\ &= 1 - (1 - \Pr(\text{a coin has } \nu = 0))^{10} \\ &= 1 - (1 - 1/2^{10})^{1000} \\ &\approx 0.63\%\end{aligned}$$

- **Conclusion**: It is probable, more than 50%

Validation vs Learning: Hoeffding Inequality

- In **validation / testing**
  - Use Hoeffding to assess how well our g (the *chosen hypothesis*) approximates f (the *unknown hypothesis*):

$$\Pr(|E_{in} - E_{out}| > \varepsilon) \leq 2\exp(-2\varepsilon^2 N)$$

    where:

$$E_{in}(g) = \frac{1}{N}\sum_i e(g(\underline{x}_i), f(\underline{x}_i))$$

$$E_{out}(g) = \mathbb{E}_{\underline{x}}[e(g(\underline{x}), f(\underline{x}))]$$

  - Since the hypothesis g is final and fixed, Hoeffding inequality guarantees that you can learn since it gives a bound for E_{out} to track E_{in}
- In **learning**
  - Need to account that our hypothesis is the best of M hypotheses, so:

$$\Pr(|E_{in} - E_{out}| > \varepsilon) \leq 2M\exp(-2\varepsilon^2 N)$$

  - The bound for E_{out} from Hoeffding is weak
- **Questions**:
  - Is the bound weak because it needs to be?
  - Is it possible to replace it with a stricter bound?

Intuition Why Bound for Hoeffding Is Weak

- The Hoeffding inequality and the union bound applied to training set

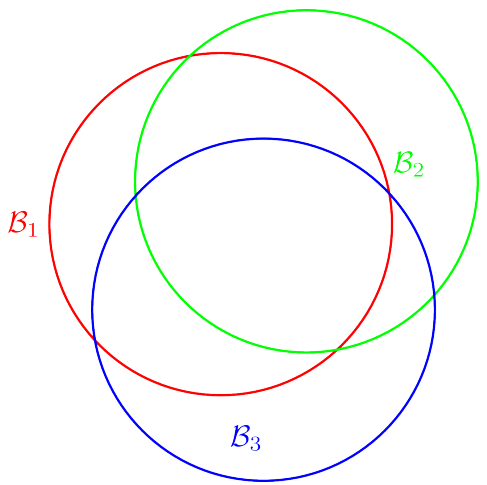
$$\Pr(|E_{in} - E_{out}| > \varepsilon) \leq 2M \exp(-2\varepsilon^2 N)$$

  is **artificially** too loose

- M was coming from the bad event:

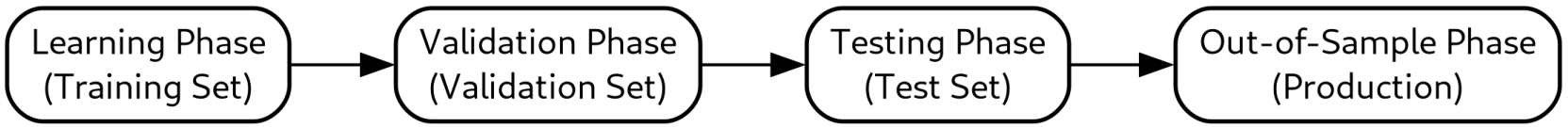
$$\begin{aligned} \mathcal{B}_i &= \textit{"hypothesis } h_i \textit{ does not generalize out-of-sample"} \\ &= "|E_{in}(h_i) - E_{out}(h_i)| > \varepsilon" \end{aligned}$$

- Since $g \in \{h_1, h_2, \cdots, h_M\}$ then $\Pr(\mathcal{B}) \leq \Pr(\bigcup_i \mathcal{B}_i) \leq \sum_i \Pr(\mathcal{B}_i)$
- The union bound assumes the events are disjoint, leading to a conservative estimate if events overlap
- **In reality**, bad events are extremely overlapping because bad hypotheses are extremely similar



Training vs Testing: College Course Analogy (1/2)

- In machine learning there are several phases



- This set-up is very similar to studying and exams in a college course
- Students study the material
  - This is the **learning phase**
- Before the final exam, students receive practice problems and solutions
  - Studying the problems improves performance by understating what they need to improve
  - This corresponds to the **validation set**

Training vs Testing: College Course Analogy (2/2)

- The final exam corresponds to the **testing phase**
  - These problems are different than the problems in the validation set
  - Why not give out exam problems to improve performance?
    - Doing well in the exam isn't the goal
    - The goal is to learn the course material
  - The final exam isn't strictly necessary
    - Gauges how well you've learned
    - Motivates you to study
    - Knowing exam problems in advance wouldn't gauge learning effectively
- What matters is how students do once they graduate and find a job
  - This is the **out-of-sample phase**

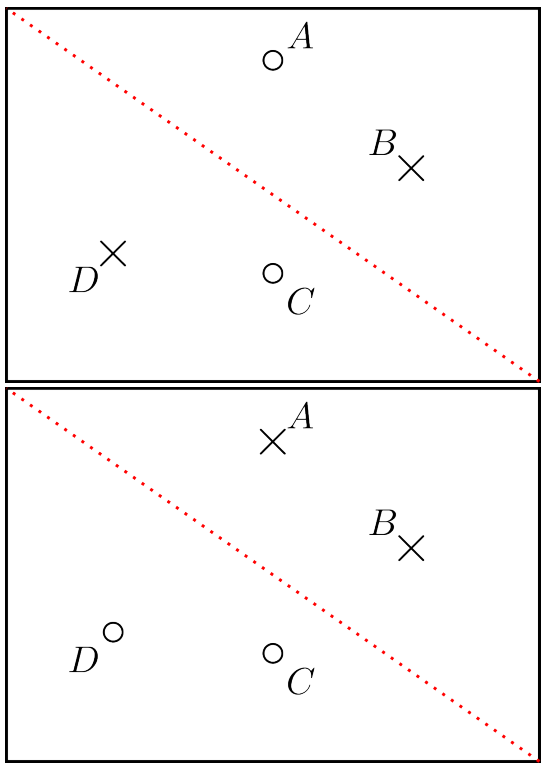
- Is Machine Learning Even Possible?
- ***Growth Function***
- The VC Dimension
- Overfitting
- Bias Variance Analysis
- Learning Curves
- Learn-Validation Approach

Dichotomy: Definition

- **Problem**: classify N (fixed) points $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N$ with an hypothesis set $\mathcal{H}$ of multi-class classifiers
- Consider an assignment D of the points to certain class $\underline{\boldsymbol{d}}_1, ..., \underline{\boldsymbol{d}}_N$
- D is a **dichotomy** for hypothesis set $\mathcal{H}$ $\iff$ there exists $h \in \mathcal{H}$ that gets the desired classification D
- **Example**
  - 4 points in a plane A, B, C, D
  - Binary classification
  - $\mathcal{H} = \{$ bidimensional perceptrons $\}$
  - Moving the separating hyperplane, you get different classifications for the points (i.e., dichotomies)

	D1	D2	D3	D4	D...
A	o	x		...	
B	x	x			
C	o	o			
D	x	o		...	

  - There are at most 2^N dichotomies
  - Certain classifications are not possible (e.g., XOR assignment)



Dichotomies vs Hypotheses

- An **hypothesis** classifies each point of $\mathcal{X}$: $\mathcal{X} \to \{-1, +1\}$
- A **dichotomy** classifies each point of a fixed set: $\{\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N\} \to \{-1, +1\}$
  - Dichotomies are "mini-hypotheses", i.e., hypotheses restricted to given points
  - A dichotomy depends on:
    - The number of points N
    - Hypothesis set $\mathcal{H}$ (i.e., the possible models)
    - Where the points are placed
    - How the points are assigned
- The **number of different dichotomies** is indicated by $|\mathcal{H}(\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N)|$
  - The number of dichotomies is always finite, since $|\mathcal{H}(\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N)| \leq N^K$
  - The number of hypotheses is usually infinite, i.e., $|\mathcal{H}| = \infty$
- The "complexity" of $\mathcal{H}$ is related to the number of hypothesis
- From the training set point of view what matters are dichotomies and not hypotheses
- Many (infinite) hypotheses can correspond to the same dichotomy

Growth Function

- The **growth function** counts the maximum number of possible dichotomies on N points for a hypothesis set $\mathcal{H}$:

$$m_{\mathcal{H}}(N) = \max_{\underline{\boldsymbol{x}}_1,\cdots,\underline{\boldsymbol{x}}_N \in \mathcal{X}} |\mathcal{H}(\underline{\boldsymbol{x}}_1, \cdots, \underline{\boldsymbol{x}}_N)|$$

- **Why growth function?**
  - The dichotomies depend on point distribution and assignment
  - The growth function considers the maximum by placing points in the most "favorable way" for the hypothesis set
- To compute $m_{\mathcal{H}}(N)$ by **brute force**:
  - Consider all possible placements of N points $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N$
  - Consider all possible assignments of the points to the classes
  - Consider all possible hypotheses $h \in \mathcal{H}$
  - Compute the corresponding dichotomy for h on $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N$
  - Count the number of different dichotomies

What Can Vary in a Dichotomy

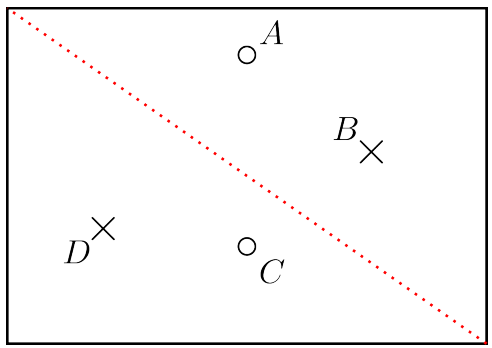
- Given:
  - An hypothesis set $\mathcal{H}$ (e.g., bidimensional perceptrons)
  - N (fixed) points $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N$
  - An assignment D of the points to certain class $\underline{\boldsymbol{d}}_1, ..., \underline{\boldsymbol{d}}_N$
- D is a **dichotomy** for hypothesis set $\mathcal{H}$ $\iff$ there exists $h \in \mathcal{H}$ that gets the desired classification D
- There are various quantities in the definition of dichotomy
  - The hypothesis set $\mathcal{H}$
    - It is fixed
  - The number of dimensions of the input space
    - It is fixed through the hypothesis set $\mathcal{H}$
  - The number of points N
    - Input to the growth function $m_{\mathcal{H}}(N)$
  - How the points are assigned to the classes $\underline{\boldsymbol{d}}_1, ..., \underline{\boldsymbol{d}}_N$
    - It is a free parameter, removed by how each hypothesis in $\mathcal{H}$ "splits" the space
  - Where the points are positioned $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N$
    - It is a free parameter, removed by the growth function through max

Growth Function Is Increasing

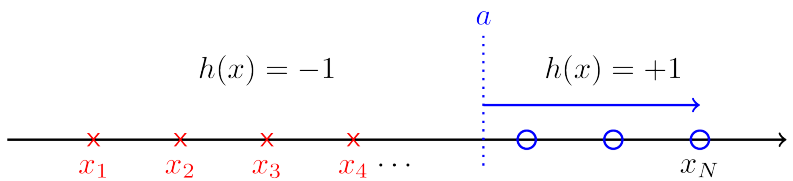
- $m_{\mathcal{H}}(N)$ increases (although not monotonically) with N
- E.g.,
  - The number of dichotomies on $N = 3$ points $m_{\mathcal{H}}(3)$ is smaller or equal than the number of dichotomies on $N = 4$ points
  - In fact we can ignore a new point and get the same classification
- $m_{\mathcal{H}}(N)$ increases with the complexity of $\mathcal{H}$
- $m_{\mathcal{H}}(N)$ increases with the number of dimensions in the input space (i.e., feature space)

Growth Function: Examples

- Consider the growth function $m_{\mathcal{H}}$ for different hypothesis sets $\mathcal{H}$
- **Perceptron on a plane**
  - $m_{\mathcal{H}}(3) = 8$
  - $m_{\mathcal{H}}(4) = 14$ (2 XOR classifications not possible)

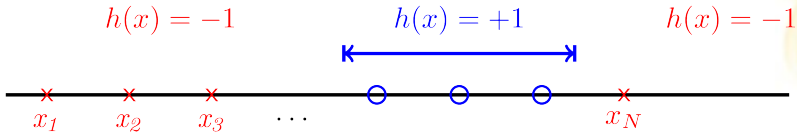


- **Positive rays** $\text{sign}(x - a)$ on $\mathbb{R}$
  - $m_{\mathcal{H}}(N) = N + 1$
  - Origin of rays a can be placed in $N + 1$ intervals

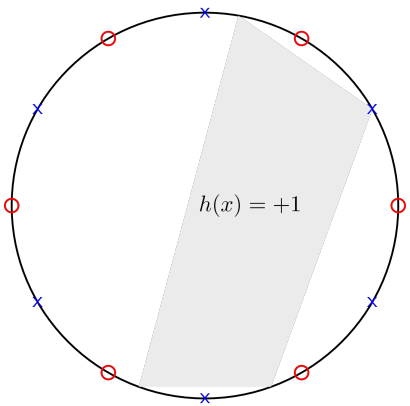


Growth Function: Examples

- **Positive intervals** on $\mathbb{R}$ $x \in [a, b]$
  - $m_{\mathcal{H}}(N) = \binom{N+1}{2} + 1 \sim N^2$
  - Pick 2 distinct intervals out of $N+1$, and there is a dichotomy with 2 points in the same interval



- **Convex sets on a plane**
  - $m_{\mathcal{H}}(N) = 2^N$
  - Place points in a circle and can classify N points in any way



Break Point of an Hypothesis Set

- Given an hypothesis set $\mathcal{H}$
- A hypothesis set $\mathcal{H}$ **shatters** N **points** $\iff$ $m_{\mathcal{H}}(N) = 2^N$
  - There is a position of N points and a class assignment that you can classify using $h \in \mathcal{H}$
  - It does not mean all sets of N points can be classified in any way
- k is a **break point** for $\mathcal{H}$ $\iff$ $m_{\mathcal{H}}(k) < 2^k$
  - I.e., no data set of size k can be shattered by $\mathcal{H}$
  - E.g.,
    - For 2D perceptron: a break point is 4
    - For positive rays: a break point is 2
    - For positive intervals: a break point is 3
    - For convex set on a plane: there is no break point

Break Point for an Hypothesis Set and Learning

- If there is a break point for a hypothesis set $\mathcal{H}$, it can be shown that:
  - $m_{\mathcal{H}}(N)$ is polynomial in N
  - Instead of Hoeffding's inequality for learning

$$\Pr(|E_{in}(g) - E_{out}(g)| > \varepsilon) \leq 2Me^{-2\varepsilon^2 N}$$

    you can use the Vapnik-Chervonenkis inequality:

$$\Pr(\text{bad generalization}) \leq 4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\varepsilon^2 N}$$

  - Since $m_{\mathcal{H}}(N)$ is polynomial in N, it will be dominated by the negative exponential, given enough examples
  - You can have a generalization bound: machine learning works!
- A hypothesis set can be characterized from the learning point of view by the **existence and value of a break point**

- Is Machine Learning Even Possible?
- Growth Function
- ***The VC Dimension***
- Overfitting
- Bias Variance Analysis
- Learning Curves
- Learn-Validation Approach

VC Dimension of an Hypothesis Set

- The **VC dimension of a hypothesis set** $\mathcal{H}$, denoted as $d_{VC}(\mathcal{H})$, is defined as the largest value of N for which $m_{\mathcal{H}}(N) = 2^N$
  - I.e., the VC dimension is the most points $\mathcal{H}$ can shatter
- **Properties** of the VC dimension: if $d_{VC}(\mathcal{H}) = N$ then
  - Exists a constellation of N points that can be shattered by $\mathcal{H}$
    - Not all sets of N points can be shattered
    - If N points were placed randomly, they could not be necessarily shattered
  - $\mathcal{H}$ can *shatter* N points for any $N \leq d_{VC}(\mathcal{H})$
  - The *smallest break point* is $d_{VC} - 1$
  - The *growth function* in terms of the VC dimension is $m_{\mathcal{H}} \leq \sum_{i=0}^{d_{VC}} \binom{N}{i}$
  - The VC dimension is the *order of the polynomial bounding* $m_{\mathcal{H}}$

VC Dimension: Interpretation

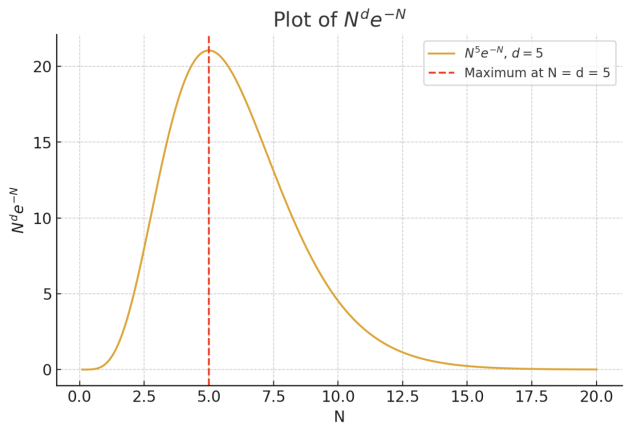
- The VC dimension **measures the complexity** of a hypothesis set in terms of **effective parameters**
- E.g.,
  - A perceptron in a d-dimensional space has $d_{VC} = d + 1$
  - In fact d_{VC} is the number of perceptron parameters!
  - E.g., for a 2D perceptron ($d = 2$), the break point is 2, so $d_{VC} = 3$
- The VC dimension considers the model as a black box in order to estimate effective parameters
  - How many points N a model can shatter, not the number of parameters
- Not all parameters contribute to degrees of freedom
  - E.g., combining N 1D perceptrons gives $2N$ parameters, but the effective degrees of freedom remain 2
- A complex hypothesis $\mathcal{H}$:
  - Has more parameters (higher VC dimension d_{VC})
  - Requires more examples for training

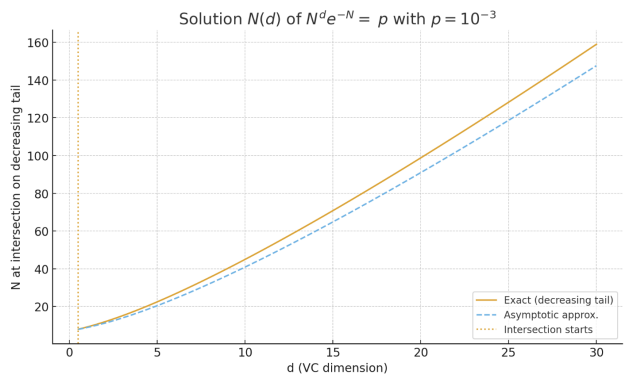
VC Generalization Bounds

- How many data points are needed to obtain $\Pr(|E_{in} - E_{out}| > \varepsilon) \leq \delta$?
- The VC inequality states

$$\Pr(\text{bad generalization}) \leq 4 m_{\mathcal{H}}(2N) e^{-\frac{1}{8}\varepsilon^2 N}$$

- $N^d e^{-N}$ abstracts the upper bound term
  - Plot $N^d e^{-N}$ vs. N: Power dominates for small N, exponential for large N and brings it to 0
  - Vary d (VC dimension) function peaks for larger N, then approaches the region of interest $\lesssim 1$
- Plot intersection of $N^d e^{-N}$ with a probability as a function of d
  - Examples N needed are proportional to d
  - Rule of thumb: $N \geq 10 d_{VC}$ for generalization





SCIENCE ACADEMY

VC Generalization Bounds

- The VC inequality

$$\Pr(|E_{in} - E_{out}| > \varepsilon) \leq 4 m_{\mathcal{H}}(2N) e^{-\frac{1}{8}\varepsilon^2 N}$$

  can be used in several ways to relate ε, δ, and N, e.g.,

- Examples
  - "Given $\varepsilon = 1\%$ error, how many examples N are needed to get $\delta = 0.05$?"
  - "Given N examples, what's the probability of an error larger than ε?"
- You can equate δ to $4 m_{\mathcal{H}}(2N) e^{\frac{1}{8}\varepsilon^2 N}$ and solve for ε, getting

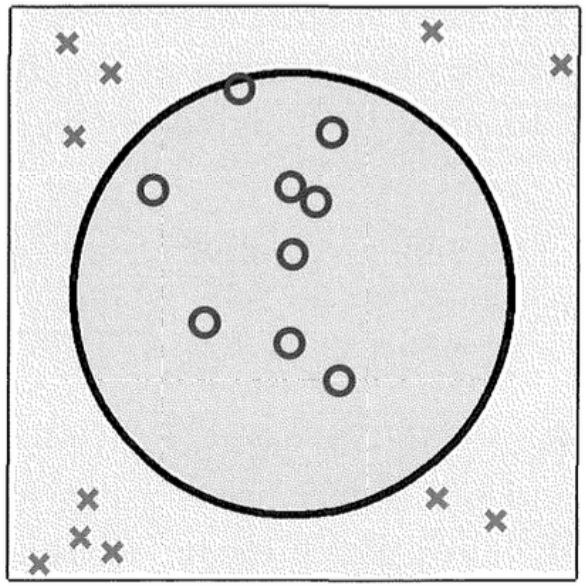
$$\Omega(N, \mathcal{H}, \delta) = \sqrt{\frac{8}{N} \ln \frac{4 m_{\mathcal{H}}(2N)}{\delta}}$$

- Then you can say $|E_{out} - E_{in}| \leq \Omega(N, \mathcal{H}, \delta)$ with probability $\geq 1 - \delta$
  - The generalization bounds are then: $\Pr(E_{out} \leq E_{in} + \Omega) \geq 1 - \delta$

How to Void the VC Analysis Guarantee

- Consider the case where data is genuinely non-linear
  - E.g., "o" points in the center and "x" in the corners
- Transform to high-dimensional $\mathcal{Z}$ with:

$$\Phi : \underline{\boldsymbol{x}} = (x_0, ..., x_d) \rightarrow \underline{\boldsymbol{z}} = (z_0, ..., z_{\tilde{d}})$$

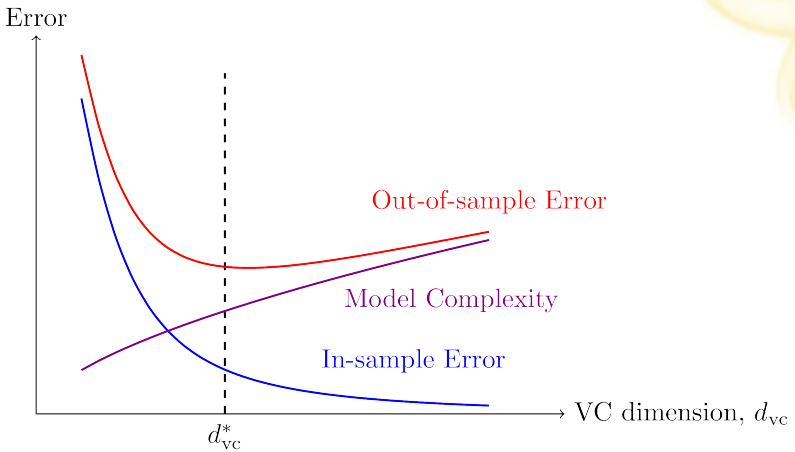


- $d_{VC} \leq \tilde{d} + 1$; smaller $\tilde{d}$ improves generalization
  - Use $\underline{\boldsymbol{z}} = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$
  - Why not $\underline{\boldsymbol{z}} = (1, x_1^2, x_2^2)$?
  - Why not $\underline{\boldsymbol{z}} = (1, x_1^2 + x_2^2)$?
  - Why not $\underline{\boldsymbol{z}} = (x_1^2 + x_2^2 - 0.6)$?
- Some model coefficients were zero and discarded, leaving machine learning the rest
  - VC analysis is a warranty, forfeited if data is examined before model selection (data snooping)
  - From VC analysis, complexity is that of the initial hypothesis set

- Is Machine Learning Even Possible?
- Growth Function
- The VC Dimension
- ***Overfitting***
- Bias Variance Analysis
- Learning Curves
- Learn-Validation Approach

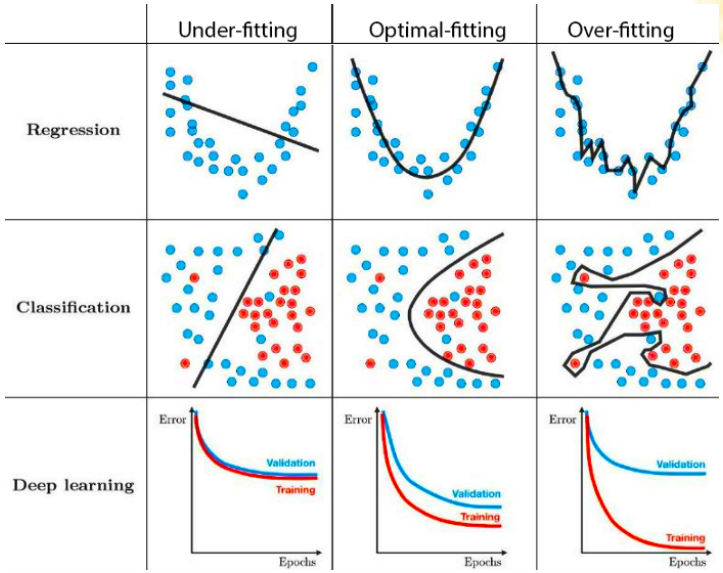
Overfitting: Definition

- **Overfitting** occurs when the model fits the data more than what is warranted
- Surpass point where E_{out} is minimal (optimal fit)
  - Model complexity too high for data/noise
  - Noise in training set mistaken for signal
- **Fitting noise instead of signal** is not useless but harmful
  - Model infers in-sample pattern that, when extrapolated out-of-sample, deviates from target function $\Longrightarrow$ poor generalization



Optimal Fit

- The opposite of overfitting is **optimal fit**
  - Train a model with proper complexity for the data
- The optimal fit:
  - Implies E_{out} is minimal
  - Does not imply generalization error $E_{out} - E_{in}$ is minimal
    - E.g., no training implies generalization error equal to 0
- The **generalization error** is the additional error $E_{out} - E_{in}$ when going from in-sample to out-of-sample



Overfitting: Diamond Price Example

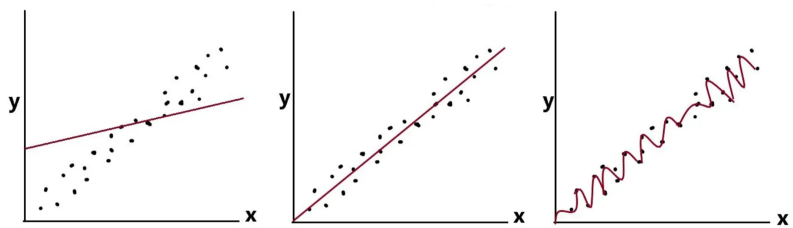
- Predict diamond price as a function of carat size (regression problem)
- **True relationship**

$$\text{price} \sim (\text{carat size})^2 + \varepsilon$$

  where:

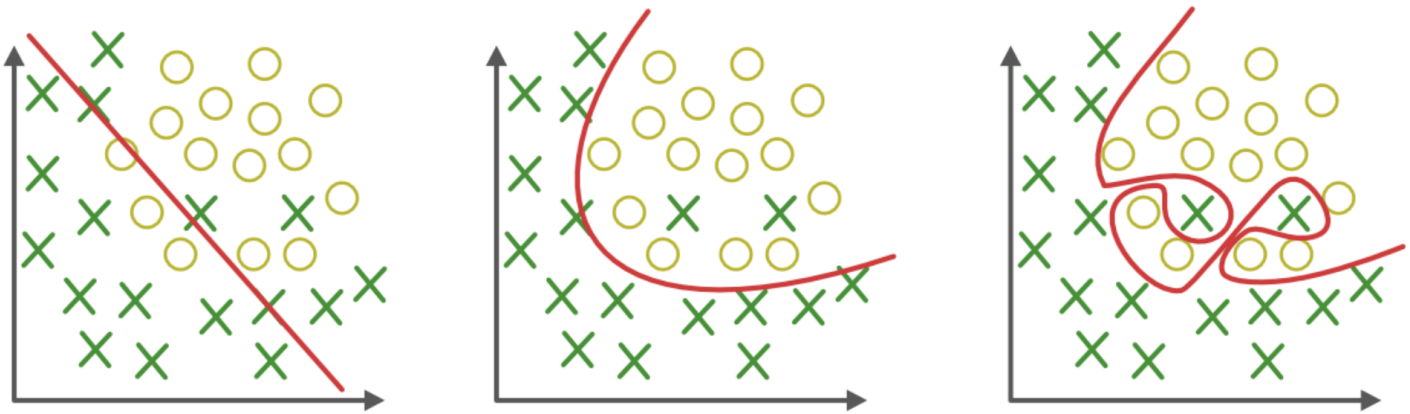
  - Square function: price increases more with rarity
  - Noise ε: e.g., market noise, missing features

- **Fit with:**
  - *Line*
    - Underfit
    - High bias (large error)
    - Low variance (stable model)
  - *Polynomial of degree 2*
    - right fit
  - *Polynomial of degree 10*
    - Overfit (wiggly curve)
    - Low bias
    - High variance (many degrees of freedom)



Overfitting: Classification Example

- Assume:
  - You want to separate 2 classes using 2 features x_1, x_2
  - The true class boundary has a parabola shape
- You can use logistic regression and a decision boundary equal to:
  - A line logit$(w_0 + w_1 x + w_2 y)$
    - Underfit
    - High bias, low variance
  - A parabola logit$(w_0 + w_1 x + w_2 x^2 + w_3 xy + w_4 y^2)$
    - Right fit
  - A wiggly decision boundary logit(w_0 + high powers of x_1, x_2)
    - Overfit
    - Low bias, high variance



- Is Machine Learning Even Possible?
- Growth Function
- The VC Dimension
- Overfitting
- ***Bias Variance Analysis***
- Learning Curves
- Learn-Validation Approach

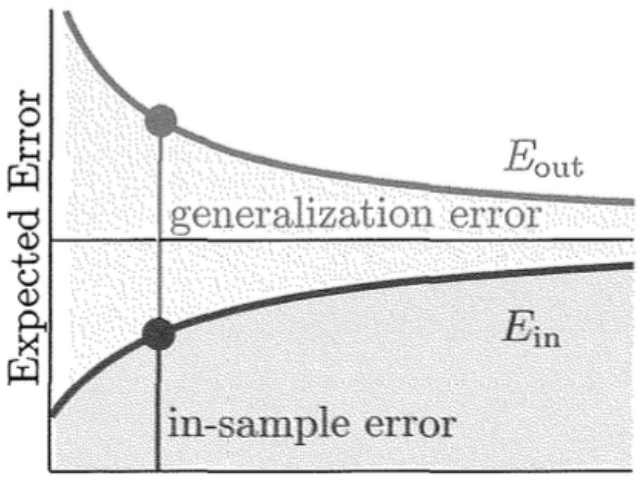
VC Analysis vs Bias-Variance Analysis

- Both VC analysis and bias-variance analysis are concerned with the hypothesis set $\mathcal{H}$
  - **VC analysis**:

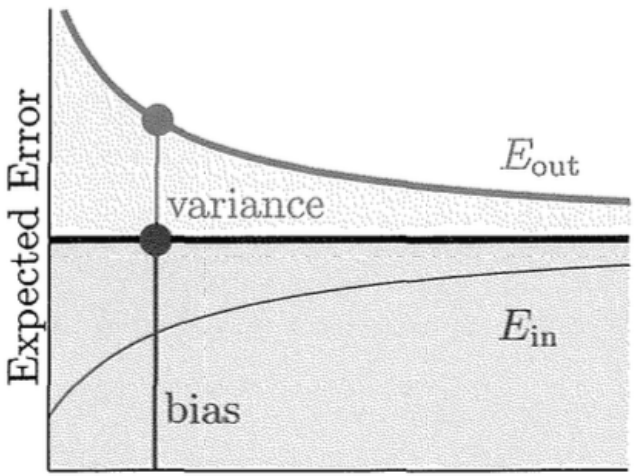
$$E_{out} \leq E_{in} + \Omega(\mathcal{H})$$

  - **Bias-variance analysis**

$$E_{out} = \text{bias} + \text{variance}$$



VC Analysis



Bias-Variance Analysis

Hypothesis Set and Bias-Variance Analysis

- **Learning** consists in finding $g \in \mathcal{H}$ such that $g \approx f$ where f is an unknown function
- The **tradeoff in learning** is between:
  - Bias vs variance
  - Overfitting vs underfitting
  - More complex vs less complex $\mathcal{H}$ / h
  - Approximation (in-sample) vs generalization (out-of-sample)

Decomposing Error in Bias-Variance (1/4)

- **Problem**
  - Regression set-up: target is a real-valued function
  - Hypothesis set $\mathcal{H} = \{h_1(\underline{x}), h_2(\underline{x}), ...h_n(\underline{x})\}$
  - Training data $\mathcal{D}$ with N examples
  - Squared error $E_out = \mathbb{E}[(g(\underline{x}) - f(\underline{x}))^2]$
  - Choose the best function $g \in \mathcal{H}$ that approximates unknown f
- **Question**
  - What is the out-of-sample error $E_{out}(g)$ as function of $\mathcal{H}$ for a training set of N examples?

Decomposing Error in Bias-Variance (2/4)

- The final hypothesis g depends on training set D, so make the dependency explicit $g^{(D)}$:

$$E_{out}(g^{(D)}) \triangleq \mathbb{E}_{\underline{x}}[(g^{(D)}(\underline{x}) - f(\underline{x}))^2]$$

- Interested in:
  - Hypothesis set $\mathcal{H}$ rather than specific h
  - Training set D of N examples, rather than a specific D
- Remove dependency from D by averaging over all possible training sets D with N examples:

$$E_{out}(\mathcal{H}) \triangleq \mathbb{E}_D[E_{out}(g^{(D)})] = \mathbb{E}_D[\mathbb{E}_{\underline{x}}[(g^{(D)}(\underline{x}) - f(\underline{x}))^2]]$$

Decomposing Error in Bias-Variance (3/4)

- Switch the order of the expectations since the quantity is non-negative:

$$E_{out}(\mathcal{H}) = \mathbb{E}_{\underline{x}}[\mathbb{E}_D[(g^{(D)}(\underline{x}) - f(\underline{x}))^2]$$

- Focus on $\mathbb{E}_D[(g^{(D)}(\underline{x}) - f(\underline{x}))^2]$ which is a function of $\underline{x}$
- Define the *average hypothesis* over all training sets as:

$$\overline{g}(\underline{x}) \triangleq \mathbb{E}_D[g^{(D)}(\underline{x})]$$

- Add and subtract it inside the $\mathbb{E}_D$ expression:

$$\begin{aligned}
E_{out}(\mathcal{H}) =& \mathbb{E}_{\underline{x}}\left[\mathbb{E}_D\left[\left(g^{(D)}(\underline{x}) - f(\underline{x})\right)^2\right]\right] \\
=& \mathbb{E}_{\underline{x}}\mathbb{E}_D[(g^{(D)} - \overline{g} + \overline{g} - f)^2] \\
=& \mathbb{E}_{\underline{x}}\mathbb{E}_D[(g^{(D)} - \overline{g})^2 + (\overline{g} - f)^2 + 2(g^{(D)} - \overline{g})(\overline{g} - f)] \\
& (\mathbb{E}_D \text{ is linear and } (\overline{g} - f) \text{ doesn't depend on } D) \\
=& \mathbb{E}_{\underline{x}}\left[\mathbb{E}_D[(g^{(D)} - \overline{g})^2] + (\overline{g} - f)^2 + 2\mathbb{E}_D[(g^{(D)} - \overline{g})](\overline{g} - f)\right]
\end{aligned}$$

Decomposing Error in Bias-Variance (4/4)

- The cross term:

$$\mathbb{E}_D[(g^{(D)} - \overline{g})](\overline{g} - f)$$

  disappears since applying the expectation on D, it is equal to:

$$(g^{(D)} - \mathbb{E}_D[\overline{g}])(\overline{g} - f) = 0 \cdot (\overline{g} - f) = 0 \cdot \text{constant}$$

- Finally:

$$\begin{aligned} E_{out}(\mathcal{H}) &= \mathbb{E}_{\underline{x}}[\mathbb{E}_D[(g^{(D)} - \overline{g})^2] + (\overline{g}(\underline{x}) - f(\underline{x}))^2] \\ &= \mathbb{E}_{\underline{x}}[\mathbb{E}_D[(g^{(D)} - \overline{g})^2]] + \mathbb{E}_{\underline{x}}[(\overline{g} - f)^2] \quad (\mathbb{E}_{\underline{x}} \text{ is linear}) \\ &= \mathbb{E}_{\underline{x}}[\text{var}(\underline{x})] + \mathbb{E}_{\underline{x}}[\text{bias}(\underline{x})^2] \\ &= \text{variance} + \text{bias} \end{aligned}$$

Interpretation of Average Hypothesis

- The **average hypothesis** over all training sets

$$\overline{g}(\underline{\boldsymbol{x}}) \triangleq \mathbb{E}_D[g^{(D)}(\underline{\boldsymbol{x}})]$$

  can be interpreted as the "best" hypothesis from $\mathcal{H}$ training on N samples
  - Note: $\overline{g}$ is not necessarily $\in \mathcal{H}$
- In fact it's like **ensemble learning**:
  - Consider all the possible data sets D with N samples
  - Learn g from each D
  - Average all the hypotheses

Interpretation of Variance and Bias Terms

- The out-of-sample error can be decomposed as:

$$E_{out}(\mathcal{H}) = \text{bias}^2 + \text{variance}$$

- **Bias term**

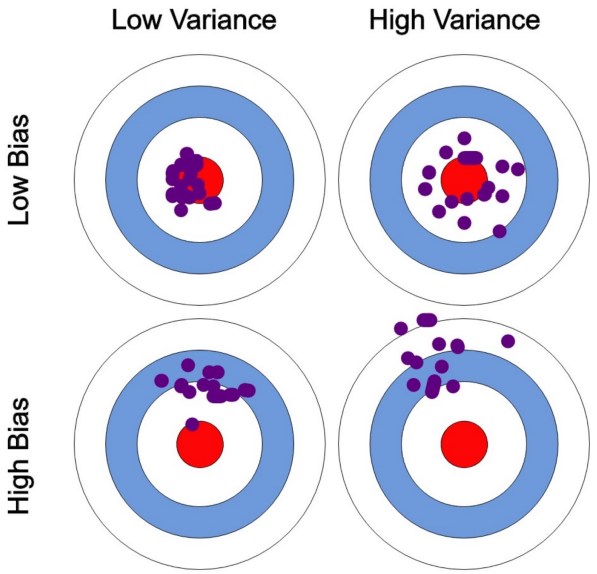
$$\text{bias}^2 = \mathbb{E}_{\underline{x}}[(\overline{g}(\underline{x}) - f(\underline{x}))^2]$$

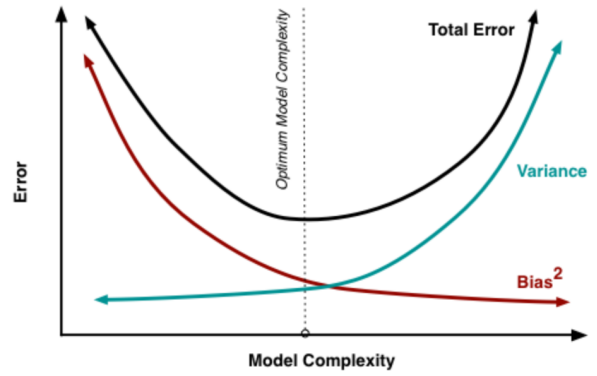
  - Does not depend on learning as it is not a function of the data set D
  - Measures how limited $\mathcal{H}$ is
    - I.e., the ability of $\mathcal{H}$ to approximate the target with infinite training sets

- **Variance term**

$$\text{variance} = \mathbb{E}_{\underline{x}}\mathbb{E}_D[(g^{(D)}(\underline{x}) - \overline{g}(\underline{x}))^2]$$

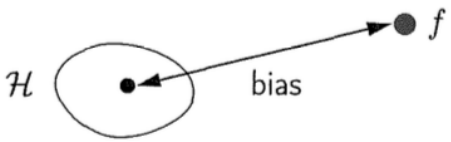
  - Measures variability of the learned hypothesis from D for any $\underline{x}$
    - With infinite training sets, we could focus on the "best" g, which is $\overline{g}$
    - But we have only one data set D at a time, incurring a cost



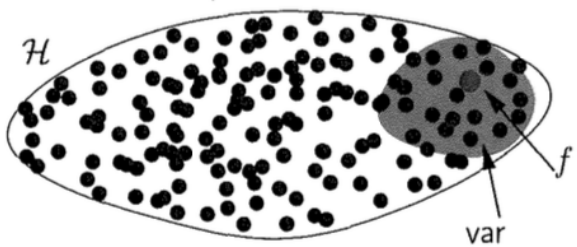


Variance and Bias Term Varying Cardinality of $\mathcal{H}$

- If hypothesis set **has a single function**:
  $\mathcal{H} = \{h \neq f\}$
  - Large bias
    - h might be far from f
  - Variance $= 0$
    - No cost in choosing hypothesis



- If hypothesis set **has many functions**:
  $\mathcal{H} = \{\text{many hypotheses } h\}$
  - Bias can be 0
    - E.g., if $f \in \mathcal{H}$
  - Large variance
    - Depending on data set D, end up far from f
    - Larger $\mathcal{H}$, farther g from f



Bias-Variance Trade-Off: Numerical Example

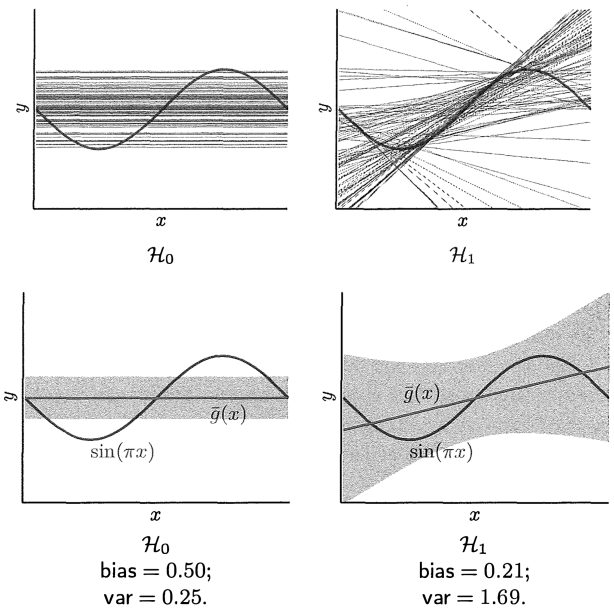
- **Machine learning problem**:
  - Target function $f(x) = \sin(\pi x), x \in [-1, 1]$
  - Noiseless target
  - You have $f(\underline{\boldsymbol{x}})$ for $N = 2$ points
- **Two hypotheses sets** $\mathcal{H}$:
  - Constant model: $\mathcal{H}_0 : h(x) = b$
  - Linear model: $\mathcal{H}_1 : h(x) = ax + b$
- **Which model is best**?
  - Depends on the perspective!
  - Best for *approximation*: minimal error approximating the sinusoid
  - Best for *learning*: learn the unknown function with minimal error from 2 points

Bias-Variance Trade-Off: Numerical Example

- **Approximation**
  - $E_{out}(g_0) = 0.5$
    - g_0 is a constant and approximates the sinusoid poorly (higher bias)
  - $E_{out}(g_1) = 0.2$
    - g_1 is a line and has more degrees of freedom (lower bias)
  - The line model *approximates better* than the constant model
- **Learning**
  - Algorithm:
    - Pick 2 points as training set D
    - Learn g from D
    - Compute $\mathbb{E}_D[E_{out}(g)]$
  - Average over all data sets D:

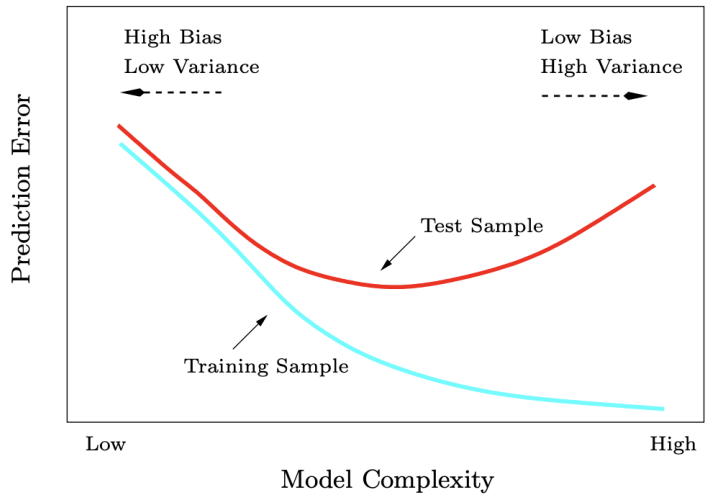
$$E_{out} = \text{bias}^2 + \text{variance}$$

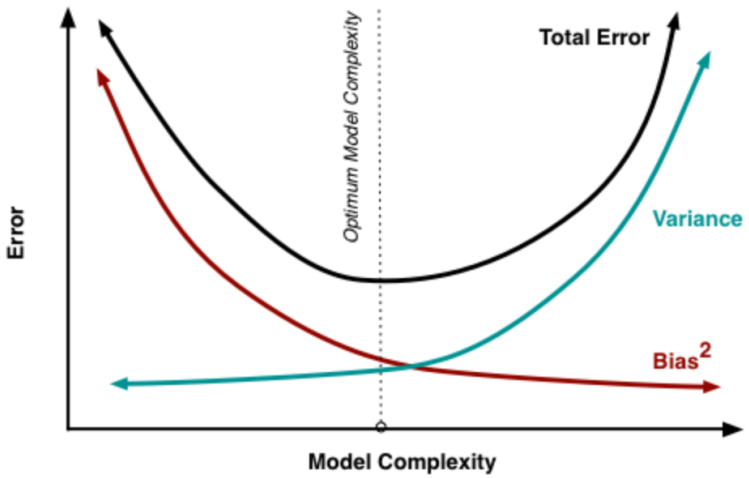
  - $E_{out}(g_0) = 0.5 + 0.25 = 0.75$
    - g_0 is more stable given the data set (lower variance)
  - $E_{out}(g_1) = 0.2 + 1.69 = 1.9$
    - g_1 heavily depends on the training set (higher variance)
  - The constant model *learns better* than the line model



Bias-Variance Curves

- **Bias-variance curves** are plots of E_{out} increasing the complexity of the model
- Typical **shape** of bias-variance curves
  - E_{in} and E_{out} start from the same point
  - E_{in}
    - Is decreasing with increasing model complexity
    - Can even go to 0
  - E_{out}
    - Is always larger than E_{in}
    - Is the sum of bias and variance
    - Has a bowl shape
    - Reaches a minimum for optimal fit
    - Before the minimum there is a "high bias / underfitting" regime
    - After the minimum there is a "high variance / overfitting" regime





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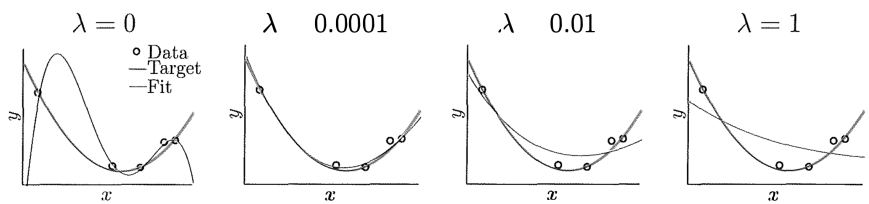
Bias-Variance Curves and Regularization

- Use **model with regularization** to learn at the same time:
  - Model coefficients $\underline{\boldsymbol{w}}$
  - Model "complexity" (e.g., VC dimension)
- Learn the optimal model $\underline{\boldsymbol{w}}(\lambda)$ as a function of $\lambda = \{..., 10^{-1}, 1.0, 10, ...\}$ by optimizing:

$$\underline{\boldsymbol{w}}(\lambda) = \text{argmin}_{\underline{\boldsymbol{w}}} E_{aug}(\underline{\boldsymbol{w}}) = E_{in}(\underline{\boldsymbol{w}}) + \Omega(\lambda)$$

- Interpret regularization parameter:
  - Small λ:
    - Complex model
    - Low bias
    - High variance
  - Large λ:
    - Simple model
    - High bias
    - Low variance
  - An intermediate λ is optimal



How to Measure the Model Complexity

- Number of features
- Parameters for model form / degrees of freedom, e.g.,
  - VC dimension d_{VC}
  - Degree of polynomials
  - k in KNN
  - ν in NuSVM
- Regularization param λ
- Training epochs for neural network

Bias-Variance Decomposition with a Noisy Target

- Extend bias-variance decomposition to **a noisy target**

$$y = f(\underline{\boldsymbol{x}}; \underline{\boldsymbol{w}}) + \varepsilon = \underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}} + \varepsilon$$

- With similar hypothesis and analysis conclude that:

$$\begin{aligned} E_{out}(\mathcal{H}) &= \mathbb{E}_{D,\underline{\boldsymbol{x}}}\left[(g^{(D)} - \overline{g})^2\right] + \mathbb{E}_{\underline{\boldsymbol{x}}}\left[(\overline{g} - f)^2\right] + \mathbb{E}_{\varepsilon,\underline{\boldsymbol{x}}}\left[(f - y)^2\right] \\ &= \text{variance} + \text{bias} + \text{stochastic noise} \end{aligned}$$

- The out-of-sample error is the sum of 3 contributions
  1. **Variance**: from the set of hypotheses to the centroid of the hypothesis set
  2. **Bias**: from the centroid of the hypothesis set to the noiseless function
  3. **Noise**: from the noiseless function to the real function

Bias as Deterministic Noise

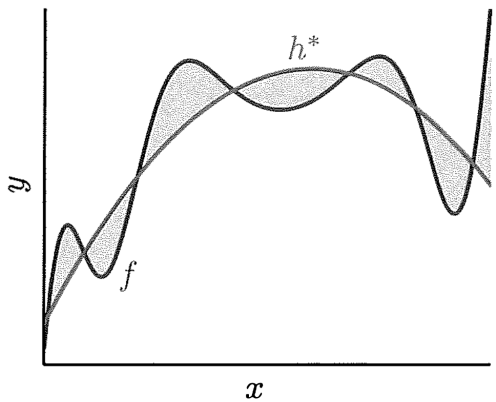
- The bias term can be interpreted as **deterministic noise**
- **Bias** is the part of the target function that hypothesis set cannot capture:

$$h^*(\underline{\boldsymbol{x}}) - f(\underline{\boldsymbol{x}})$$

where:

  - $h^*()$ is the best approximation of $f(\underline{\boldsymbol{x}})$ in the hypothesis set $\mathcal{H}$ (e.g., $\overline{g}(x)$)

- The hypothesis set $\mathcal{H}$ cannot learn the deterministic noise since it is outside of its ability, and thus it behaves like "noise"

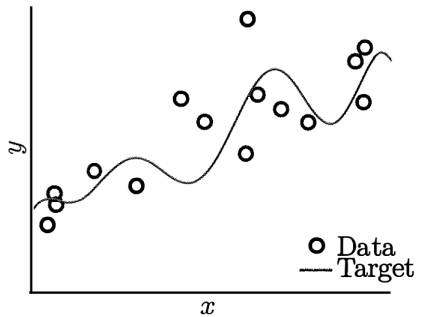


Deterministic vs Stochastic Noise in Practice

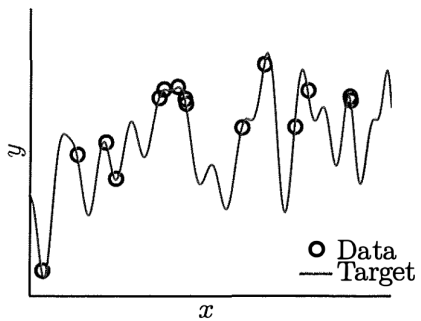
- **Deterministic noise:**
  - Fixed for a particular $\underline{\boldsymbol{x}}$
  - Depends on $\mathcal{H}$
  - Independent of ε or D
- **Stochastic noise:**
  - Not fixed for $\underline{\boldsymbol{x}}$
  - Independent of D or $\mathcal{H}$
- In a machine learning problem, no difference exists between stochastic and deterministic noise, as $\mathcal{H}$ and D are fixed
  - From the training set alone, you cannot determine if data is from a *noiseless complex* target or a *noisy simple* target

Deterministic vs Stochastic Noise Example

- **Two targets**:
  - Noisy low-order target (10th order polynomial)
  - Noiseless high-order target (50th order polynomial)
- **Training set**
  - Generate $N = 15$ data points
- **Two models**
  - $\mathcal{H}_2$ low-order hypothesis (2nd order polynomial)
  - $\mathcal{H}_{10}$ high-order hypothesis (10th order polynomial)
- Learning model:
  - Sees only training samples
  - Can't distinguish noise sources



(a) 10th order target function

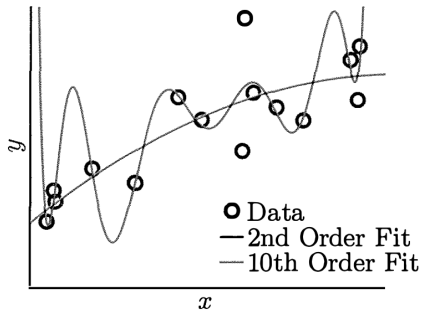


(b) 50th order target function

Deterministic vs Stochastic Noise Example

- Noisy low-order target:
  - Fit 2nd to 10th order polynomial
  - $\downarrow E_{in}$ (more degrees of freedom), $\uparrow\uparrow E_{out}$ (fits noise)
- Noiseless high-order target
  - Fit 2nd to 10th order polynomial
  - Same phenomenon
  - $\downarrow E_{in}$ (more degrees of freedom), $\uparrow\uparrow E_{out}$ (fits noise)
- **Wrong approach**
  - Target is 10th order polynomial
  - Use 10-order hypothesis to fit target perfectly
- **Right approach**
  - Consider number of data points, i.e., 15 points
  - Rule of thumb from VC analysis

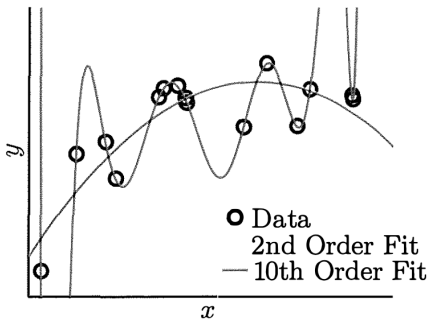
    degrees of freedom of model = number of data point
  - Use 1 or 2 degrees of freedom



(a) Noisy low order target

10th order noisy target

	2nd Order	10th Order
E_{in}	0.050	0.034
E_{out}	0.127	**9.00**



(b) Noiseless high order target

50th order noiseless target

	2nd Order	10th Order
E_{in}	0.029	10^{-5}
E_{out}	0.120	**7680**

Amount of Data and Model Complexity

- One must match the *model complexity* to
  - **Data resources**
  - **Signal to noise ratio**
  - **Not target complexity**
- The rule of thumb is:

$$d_{VC}(\text{degrees of freedom of the model}) = N(\text{number of data points})/10$$

  - In other words, 10 data points needed to fit a degree of freedom
  - If the data is noisy, you need even more data

Overfitting as a Function of Data Resources, Model Complexity, Noise

- You can measure overfitting in terms of **generalization error** $\frac{E_{out} - E_{in}}{E_{out}}$
  - $\uparrow$ data resources $N \implies \downarrow$ overfitting
  - $\uparrow$ model complexity $d_{VC} \implies \uparrow$ overfitting
  - $\uparrow$ deterministic noise (target complexity) $\implies \uparrow$ overfitting
  - $\uparrow$ stochastic noise $\sigma^2 \implies \uparrow$ overfitting

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Learning Curves vs Bias-Variance Curves

- **Learning curves** are the dual of the bias-variance curves
- For **bias-variance curves**

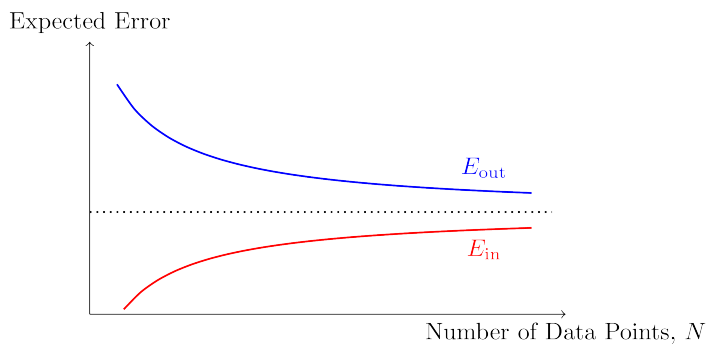
$$E_{in}, E_{out} = f(d_{VC}|N)$$

  - Keep the complexity of training set fixed (number of examples N)
  - Vary the model in terms of:
    - Model complexity d
    - Number of features p
    - Regularization amount λ

- For **learning curves**

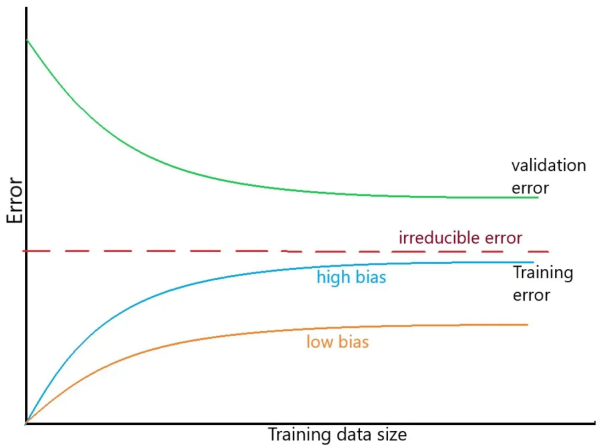
$$E_{in}, E_{out} = f(N|d_{VC})$$

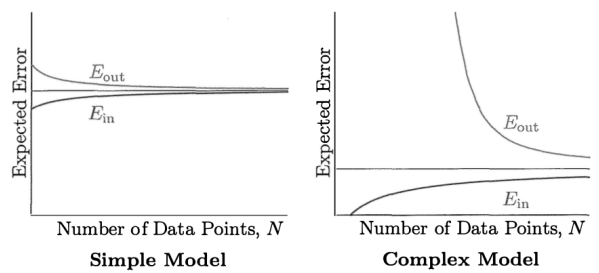
  - Fix the model
  - Vary the size N of training set



Typical Form of Learning Curves

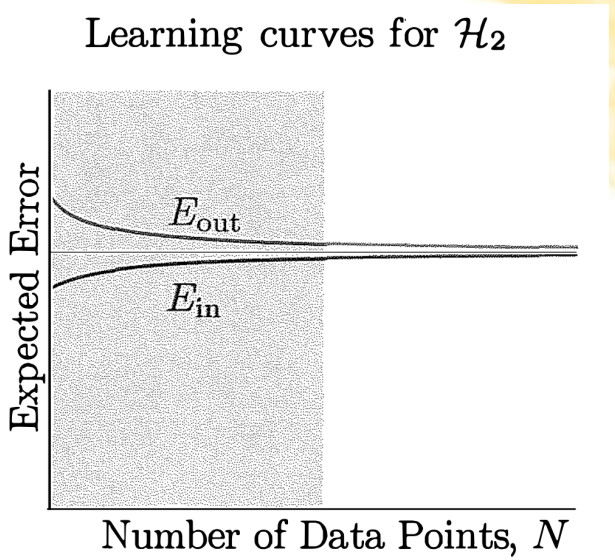
- Learning curves plot E_{in} and E_{out} as a function of data amount N, given the model $h()$
  - $E_{out} \geq E_{in}$ for any N
- **Small N**
  - E_{in} is small (even 0)
  - The model is likely overfitted, memorizing and generalizing poorly
  - E_{out} is large
- **Increasing N**
  - $E_{in} \uparrow$ as the model cannot fit all data
  - $E_{out} \downarrow$ as the model fits better and generalizes better
  - Generalization error $E_{out} - E_{in} \downarrow$
- $N \to \infty$
  - E_{in} reaches a maximum (irreducible error)
  - E_{out} reaches a minimum
  - $E_{out} - E_{in}$ depends on the complexity of the model

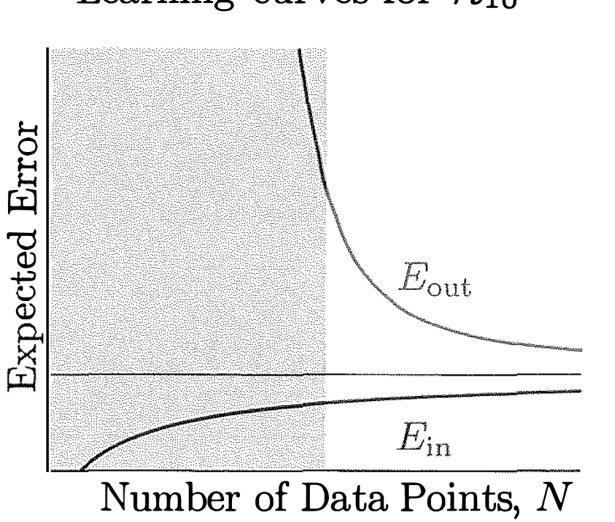




High-Bias vs High-Variance Regime

- From the learning curve you can see the two regimes:
  - **High-variance regime** for small N
    - E_{in} is small
    - Small data set $D \implies$ high dependency on D
  - More data helps reduce gap between E_{in} and E_{out}
  - **High-bias regime** for large N
    - E_{in} is large; flattens for large N
    - Best model fitted; more data won't help
    - E_{out} can be close to E_{in} (good generalization) or not





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  - Cross-Validation

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Estimating Out-Of-Sample Error with One Point

- Pick a **single out-of-sample point** $(\underline{\boldsymbol{x}}', y)$
- The error of the model h is:

$$E_{val}(h) = e(h(\underline{\boldsymbol{x}}'), y)$$

  where the error can be:

  - Squared error $(h(\underline{\boldsymbol{x}}) - y)^2$
  - Binary error $I[h(\underline{\boldsymbol{x}}) - y]$
  - ...

- The **error on an out-of-sample point** is an **unbiased estimate** of E_{out}, since:

$$\mathbb{E}[E_{val}(h)] = \mathbb{E}[e(h(\underline{\boldsymbol{x}}), y)] = E_{out}$$

- The quality of the estimate depends on the standard error $\mathbb{V}[e(h(\underline{\boldsymbol{x}}), y)]$, which in an unknown value

Estimating Out-Of-Sample Error with K Points

- To improve the estimate, use a validation set with K points $(\underline{\boldsymbol{x}}_1, y_1), ..., (\underline{\boldsymbol{x}}_K, y_K)$ drawn IID
- Compute the **error on the validation set** as:

$$E_{val}(h) = \frac{1}{K} \sum_{i=1}^{K} e(h(\underline{\boldsymbol{x}}_i), y_i)$$

- The validation error is an **unbiased estimate** of out-of-sample error since:

$$\mathbb{E}[E_{val}(h)] = E_{out}(h)$$

- The standard error is $\sqrt{K}$ smaller:

$$\mathbb{V}[E_{val}(h)] = \frac{1}{K^2} \sum_{i} \mathbb{V}[e(h(\underline{\boldsymbol{x}}_i), y_i)] + \text{covariances}$$

(covariances are 0 because $\underline{\boldsymbol{x}}_i$ independent)

$$= \frac{1}{K^2} \sum_{i} \mathbb{V}[e(h(\underline{\boldsymbol{x}}_i), y_i)]$$

$$= \frac{K\sigma^2}{K^2} = \frac{\sigma^2}{K}$$

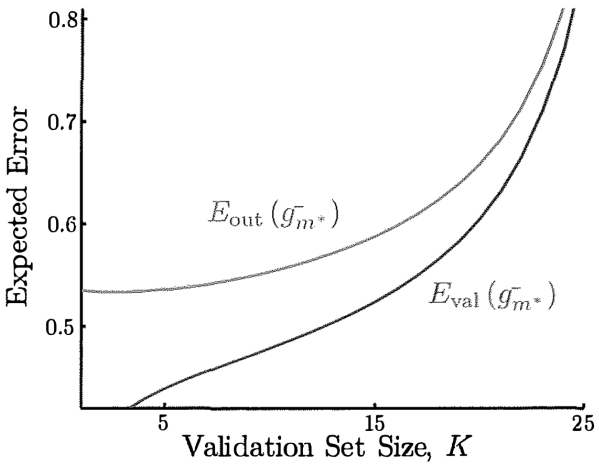
Trade-Off Between Training and Validation Set

- **Problem**: you have finite amount of data points N

$$D_{val} = \{K \text{ points}\}$$
$$D_{train} = \{N - K \text{ points}\}$$

- You know that:

$$\uparrow K \implies |E_{val} - E_{out}| \downarrow \text{ (most reliable estima}$$
$$\implies \downarrow N - K \implies E_{in}, E_{out} \uparrow \text{ (worse mc}$$



  - If K is too big, you get a **reliable estimate of a bad number**!

- **Solution**:
  - Rule of thumb: 70-30 or 80-20 split between train and validation

Error From VC Analysis vs Learn-Validation Approach

- In general:

$$E_{out}(h) = E_{in}(h) + \text{generalization error}$$

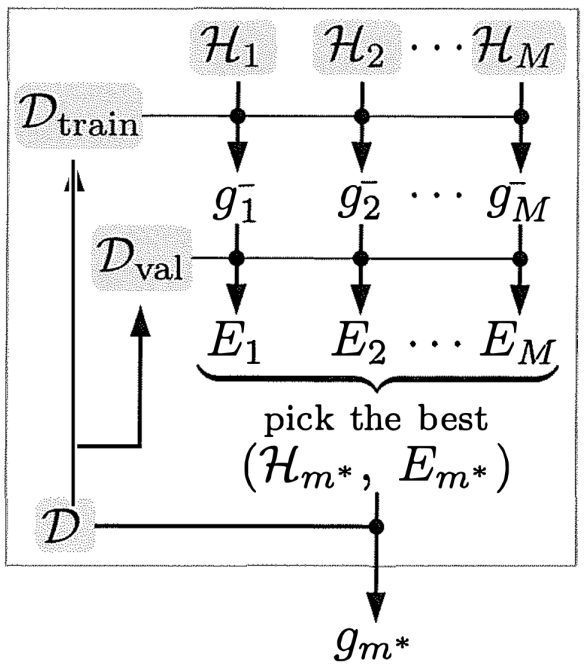
- **VC analysis**
  - Estimates generalization error as "overfit penalty" in terms of hypothesis set complexity
- **Learn-validation**
  - Estimates E_{out} directly by holding out data as validation set:

$$E_{val} \approx E_{out}$$

  - Use learn-validation approach at different points of the modeling flow:
    - For selecting hyperparameters (validation set)
    - To estimate final performance (test set)

Reusing Validation / Test Set for Training

- Any data used for learning (e.g., model training or model selection)
  - Is biased and optimistic
  - Cannot used to assess the learned model
- **Never use** D_{val} / D_{test} for training or D_{train} for evaluation
- After research is done, all available data can be used to learn
- **Algorithm**
  1. Train with $N - K$ points to learn g^-
  2. Use K points to compute $E_{val}[g^-]$ estimating $E_{out}[g^-]$
  3. Once the model form is finalized, use all N data points (including validation, test set) to re-train to get g
     - $E_{val}[g] < E_{val}[g^-]$ since g is learned on a larger data set than g^- and is thus better
  4. Deliver to customers:
     - Final hypothesis g
     - Upper bound of out-of-sample performance $E_{val}[g^-]$



Learn-Validation Approach: Pros and Cons

- **Pros**
  - Estimate E_{out} using E_{val}
  - Simple to compute, no complexity from VC analysis
- **Cons**
  - Cannot use all data for learning and validation; need a compromise
  - Learned model and E_{val} depend on the split; different splits can give different results

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Cross-validation

- **Divide dataset** into K folds, each with $\frac{N}{K}$ samples
  - Each fold should reflect dataset statistics
  - E.g., stratified sampling
- **Do K iterations** $i = 1, ..., K$
- In i-th iteration
  - Train on all folds except i using $\frac{K-1}{K}N$ points and get $g^{(-i)}(\underline{x})$
  - Validate on i-th fold using $\frac{N}{K}$ points to compute

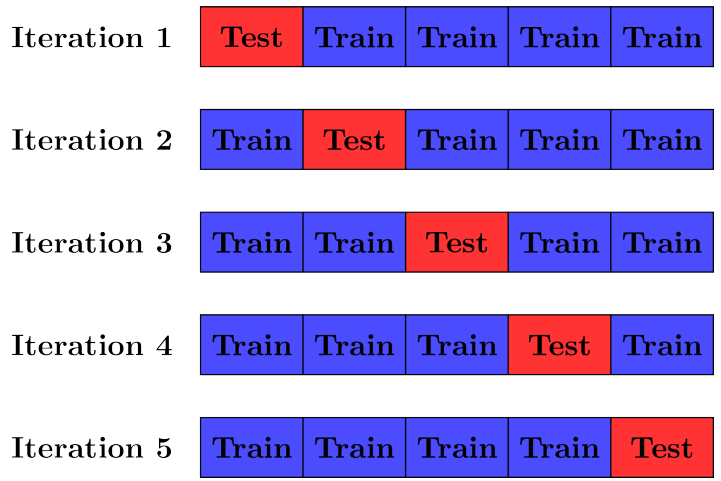
$$E_{val}^{(i)} = E_{val}[g^{(-i)}(\underline{x})]$$

- **Average** K error rates and compute bounds:

$$E_{val} = \frac{1}{K}\sum_{i} E_{val}^{(i)}$$

Train / test validation

5x cross-validation



Cross-Validation: Pros and Cons

- **Pros**
  - Efficient data usage
    - All data used for learning and validation
  - Better estimate of E_{val} than separate training/validation sets
  - Folds can be stratified
- **Cons**
  - Computationally intensive: K learning phases
  - Dependency on fold selection
  - Errors E_{val} are not independent
    - Coupling through common training samples
    - Experimentally not completely correlated

Repeated Cross-Validation

- **Repeated Cross-Validation**
  - Cross-validation results depend on fold selection
  - To remove this dependency, repeat cross-validation multiple times (e.g., 10) and average results
  - Note that *"10x 10-fold cross-validation"* is different than *"1x 100-fold cross-validation"*

Leave-One-Out Cross-Validation

- **Leave-one-out** (LOO) cross-validation
  - There are N training sessions
  - Each session trains on $N-1$ points and validates on 1 point
  - Equivalent to "N-fold cross-validation" where N is the number of examples in the dataset
- **Train**
  - For i-th fold, $N-1$ samples for training $\implies g^{(-i)} \approx g$
- **Validate**
  - Estimate the validation error on a single point (bad):

$$E_{val}[g^{(-i)}] = e(g^{(-i)}(\underline{\boldsymbol{x}}_i), y_i) \not\approx E_{out}[g^{(-i)}]$$

  - Average E_{val} over the points as estimate of E_{out} (good):

$$E_{val} = \frac{1}{N}\sum_{i=1}^{K} E_{val}[g^{(-i)}]$$

Leave-One-Out Cross-Validation: Pros and Cons

- **Pros**
  - Max data used for training
  - Deterministic procedure
    - No dependency on fold selection
- **Cons**
  - High computational cost (as many learning phases as data points)
  - Cannot be stratified
  - Higher correlation between cross-validation estimates

Bootstrap

- **Algorithm**
  - Pick N samples with replacement from a data set with N instances to build training set
  - Pick the elements never chosen to build the test set ("out-of-bag" samples)
  - Training set contains 63.2% of all the samples, 36.8% in the test set
- **Pros**
  - Works for small data sets since it "expands" the data
- **Cons**
  - Not flexible
  - Smaller percentage of instances are used for training set than 10-fold cross validation

Bootstrap: Problem

- **Assumption**
  - Given $X \sim F$
  - Draw n IID samples X_i from F
- **Goal**:
  - Consider a sampling statistic $T = g(X_1, ..., X_n)$
    - E.g., mean, median, OLS coefficients, ...
  - You want to:
    - Estimate distribution of T, e.g., $F_T(x), f_T(x)$
    - Estimate a statistic of T, e.g., mean, std err
    - Construct confidence intervals, e.g., $\mu \pm \epsilon$
    - Calculate standard errors, e.g., $\sigma(\hat{T}_n)$
    - Hypothesis testing

Bootstrap Procedure: Algorithm

- Use observed data $X_1, ..., X_n$ to construct estimated population distribution $\hat{F}_n$
- Repeat B times:
  - Draw n samples with replacement from estimated population distribution $\hat{F}_n$
  - Sampling with replacement from X_i equals sampling from $\hat{F}_n$
  - Compute sample statistics from n samples: $T^{(i)} = g(X_1^{(i)}, ..., X_n^{(i)})$
- Use B samples of $T^{(i)}$ to estimate empirical distribution $\hat{T}$
- Compute statistics (e.g., confidence interval, standard error) of T from empirical distribution of $\hat{T}$

Bootstrap: Pros

- **Tremendously useful tool**
  - Fewer assumptions
    - No need for simplifying assumptions for closed formulas
    - Data doesn't need to be Gaussian
  - Generality
    - Applies to any sample statistics, even non-linear ones (e.g., median)
- **Math $\rightarrow$ simulation**
  - Bootstrap is a non-parametric method
  - Does not rely on large sample sizes, e.g., Central Limit Theorem (CLT) / Law Large Numbers (LLN)
  - Bootstrap frees data scientists from complex math, approximations, and asymptotics

Bootstrap: Example of Die Rolls

- **Problem**
  - Compute distribution of sum of rolling a die 50 times

$$Y = \sum_{i=1}^{50} X_i = g(X_1, ..., X_{50})$$

  - Sample statistics similar to sample mean, but can be anything
- **Solution**
  1. **By math**
     - If you know PMF of the die, compute distribution using mathematics
     - Theorem of lazy statistician for mean, variance
     - Compute PDF of Y by convolving PDFs
  2. **By sampling** (real or simulated)
     - Roll die 50 times
     - Compute sample statistic
     - Repeat procedure
     - Plot approximate distribution of Y
  3. If only 50 samples of die are known $\rightarrow$ **bootstrap**

Bootstrap of the Median: Pseudo-Code

```
def bootstrap_median(x, n_boot):
    # Compute n_boot sample statistics.
    median_boot = [0.0] * n_boot
    for i in range(n_boot):
        # Sample with replacement.
        x_star = sample with replacements from x
        # Compute median for bootstrapped samples.
        median_boot[i] = median(x_star)
    # Compute mean and std err from approximation of sample statistics.
    m_median = numpy.mean(median_boot)
    se_median = numpy.std(median_boot)
    return m_median, se_median
```

Bootstrap for variance of sample statistics: explanation

- Under the hypotheses of bootstrap:
  - $X \sim F$
  - n samples X_i IID from F
  - Statistic $T = g(X_1, ..., X_n)$
  - Compute $\mathbb{V}_F[T]$ (variance of sample statistics), where F is unknown
- **First approximation**
  - Only samples from F available
  - Approximate F with $\hat{F}$, as empirical CDF $\hat{F}$ converges to F

$$\mathbb{V}_F[T] \approx \mathbb{V}_{\hat{F}}[T]$$

  - Approximation
    - Not small
    - Depends on sample size and shape of F
- **Second approximation**
  - Exact $\hat{F}$ may lack closed formula for $\mathbb{V}_{\hat{F}}[T]$
  - Use LLN and simulation to approximate variance:

$$\mathbb{V}_{\hat{F}}[T] \approx v_{boot} = \frac{1}{B}\sum_i (T_i - \overline{T})^2$$

  - Approximation size reduced by increasing B