CSE 417T
Introduction to Machine Learning

Review of Exam 1

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Logistics: Exam 1

- Exam 1 Date: March 10, 2020 (Thursday)
  - In-class exam (the same time/location as the lecture)
  - Exam duration: 75 minutes
  - Planned exam content: LFD Chapter 1 to 5
    - Everything in textbook/lectures are included, except for parts labeled as “safe to skip”.

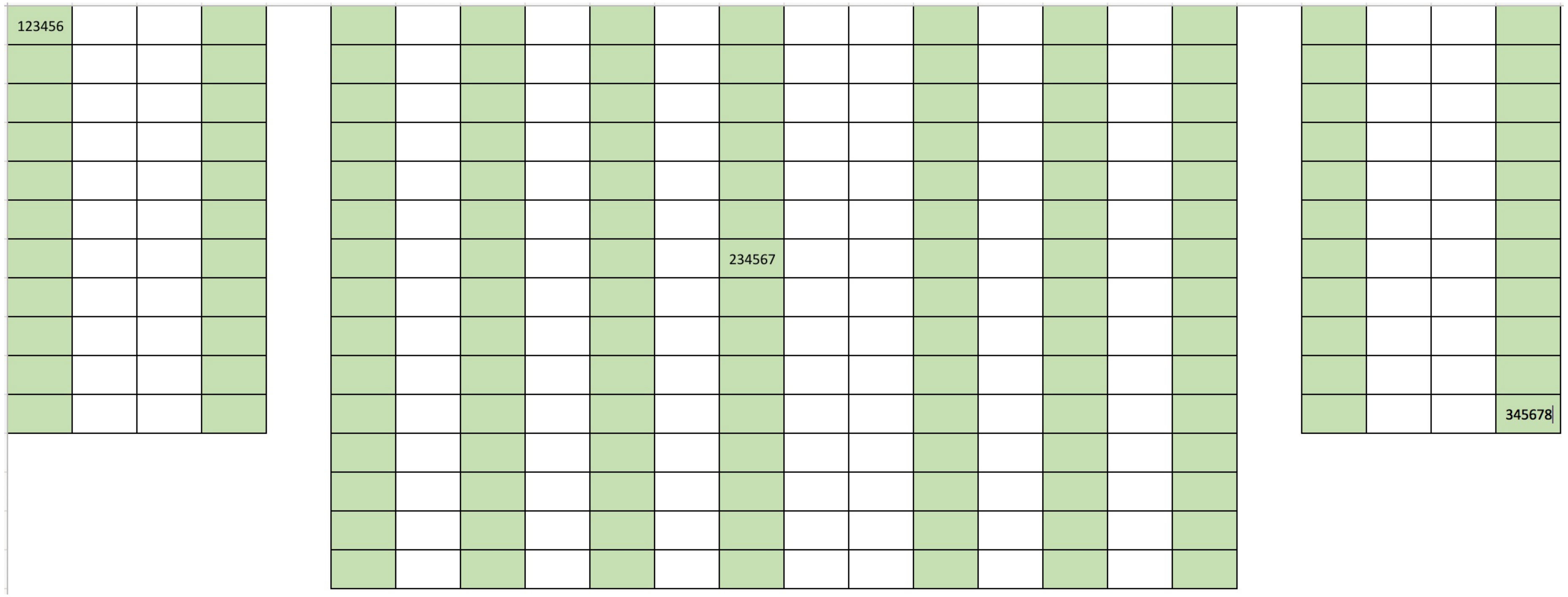
  - 2 sections of questions
    - ~5 long questions (written response questions with explanations required)
    - 10 multiple choice questions (no explanations needed)

  - Closed-book exam. You can bring two cheat-sheets
    - Up to letter size, front and back (up to 4 pages)
    - No format limitations (it can be typed, written, or a combination)

  - No calculators (you don’t need them)

Logistics: Exam Policies

- I might arrange random seat assignments
  - Will be announced on Piazza the night before the exam if I do



Logistics: Exam Policies

- Please arrive on time. No extensions will be given if you arrive late.

- During the exam, if you have a question or if you finish before time is up:
  - **Do not get up**
  - Raise your hand and I will come to you
  - I most likely will not answer questions to individual students
    - But I'll give clarifications to everyone if multiple students ask the same question

- When time is called:
  - **Stop writing**
  - **Do not get up**
  - We will come around and collect your exam

Homework

- Solution Sketch of HW2/HW3 has been posted on Gradescope
  - Not intended to be comprehensive
- Requests for extensions
  - The answer is no by default
    - Exception: documented medical/family emergencies

Plans for Today

- A summary of the content of Exam 1.
- Discussion of the practice questions.
- Discussion of any other questions you might have.

Review for Exam 1

Brief overview on the content.

Not comprehensive and not covering everything that could appear in the exam.

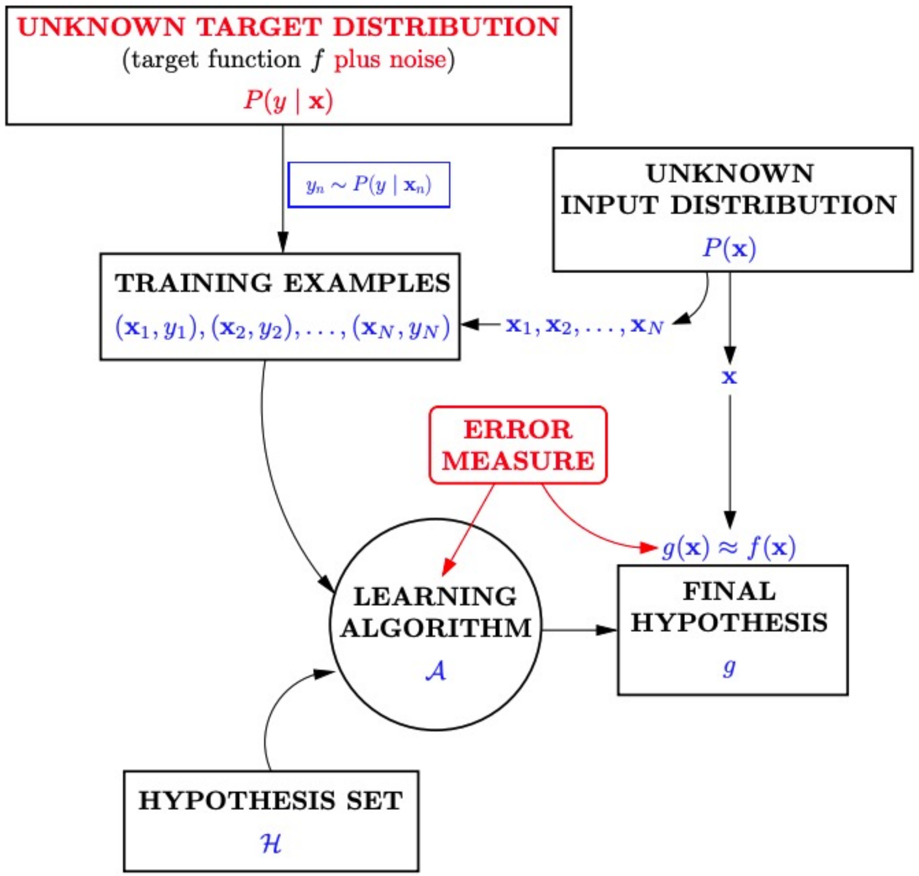
Please make sure you still study for LFD Chapter 1-5.

Let me know if you find mistakes in lecture notes.

Whenever you have doubts on the lecture notes, please use the textbook for the confirmation.

- Chap 1: Setting up the learning problem
    - Problem setup
    - probability assumptions/inferences
    - error and noise
- Chap 2: Theory of generalization (training v.s. testing)
    - Hoeffding's inequality
    - VC theory
    - Bias-variance decomposition
- Chap 3: Linear models
    - Linear classification/regression
    - logistic regression, gradient descent
    - nonlinear transformations
- Chap 4: Overfitting
    - Overfitting
    - Regularization and validation
- Chap 5: Three learning principles
    - Occam's razor, sampling bias, data snooping

Setup of the Learning Problem



- Key assumption:
  - Training/testing data from the same distribution
- Define (point-wise) error measure:
  - Binary error $e(h(\vec{x}), y) = \mathbb{I}[h(\vec{x}) \neq y]$
  - Squared error $e(h(\vec{x}), y) = (h(\vec{x}) - y)^2$
  - Cost matrix

		f: $+1$	f: -1
h	$+1$	0	1
	-1	10	0

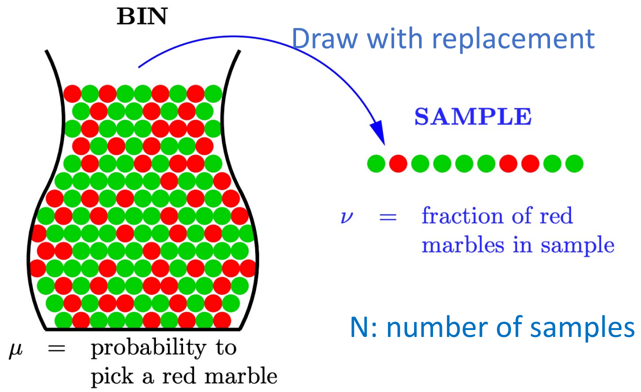
Supermarket

		f: $+1$	f: -1
h	$+1$	0	1000
	-1	1	0

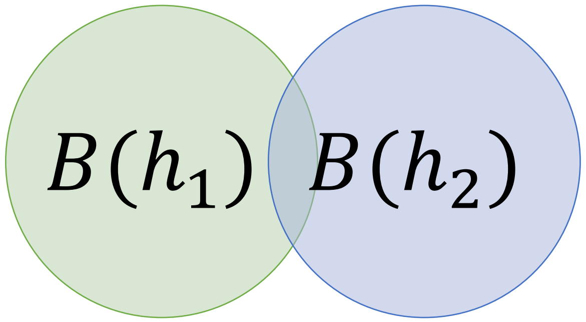
CIA

Hoeffding's Inequality

- Single hypothesis bound
  - Fix a hypothesis h
    - $E_{in}(h) = \frac{1}{N}\sum_{n=1}^{N} e(h(\vec{x}_n), y_n)$ = In-sample error of h
    - $E_{out}(h) = \mathbb{E}_{\vec{x}}[e(h(\vec{x}), y)]$ = Out-of-sample error of h
    - Hoeffding's inequality: $\Pr[|E_{out}(h) - E_{in}(h)| > \epsilon] \leq 2e^{-2\epsilon^2 N}$



- Multi-Hypothesis bound
  - Learn a g from a finite hypothesis set $H = \{h_1, \ldots, h_M\}$
    - $\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$



Dealing with Infinite Hypothesis Set: $M \to \infty$

- Instead of # hypothesis, counting "effective" # hypothesis
- Dichotomy
  - Informally, consider it as "data-dependent" hypothesis
  - Characterized by both H and N data points $(\vec{x}_1, \dots, \vec{x}_N)$

$$H(\vec{x}_1, \dots \vec{x}_N) = \{h(\vec{x}_1), \dots, h(\vec{x}_N) | h \in H\}$$

  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \dots, \vec{x}_N$

- Growth function
  - Largest number of dichotomies H can induce across all possible data sets of size N

$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

Why Growth Function?

- Finite-hypothesis Bound

  With prob at least $1 - \delta$,

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{1}{2N} ln \frac{2M}{\delta}}$$

- VC Generalization Bound (VC Inequality, 1971)

  With prob at least $1 - \delta$

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4m_H(2N)}{\delta}}$$

If we know the growth function $m_H(N)$ of H, we can obtain the learning guarantee for algorithms operating on H.

Bounding Growth Functions

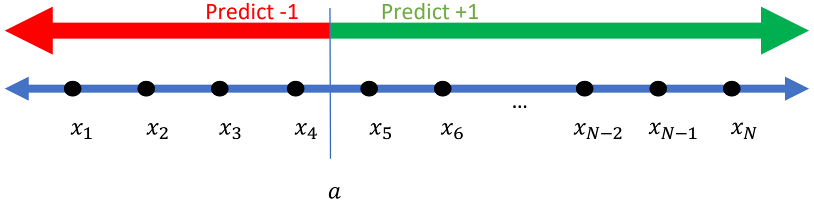
- More definitions….
  - Shatter
    - H **shatters** $(\vec{x}_1, \dots, \vec{x}_N)$ if $|H(\vec{x}_1, \dots, \vec{x}_N)| = 2^N$
    - H can induce all label combinations for $(\vec{x}_1, \dots, \vec{x}_N)$
  - Break point
    - k is a **break point** for H if no data set of size k can be shattered by H
    - k is a break point for $H \leftrightarrow m_H(k) < 2^k$
  - VC Dimension: $d_{vc}(H)$ or d_{vc}
    - The VC dimension of H is the largest N such that $m_H(N) = 2^N$
    - Equivalently, if k^* is the smallest break point for H, $d_{vc}(H) = k^* - 1$

Examples

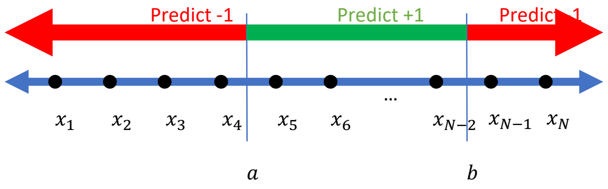
$\boldsymbol{m_H(N)}$

	N=1	N=2	N=3	N=4	N=5	Break Points	VC Dimension
Positive Rays	2	3	4	5	6	$k = 2,3,4,\ldots$	1
Positive Intervals	2	4	7	11	16	$k = 3,4,5,\ldots$	2
Convex Sets	2	4	8	16	32	None	∞
2D Perceptron	2	4	8	14	?	$k = 4,5,6,\ldots$	3

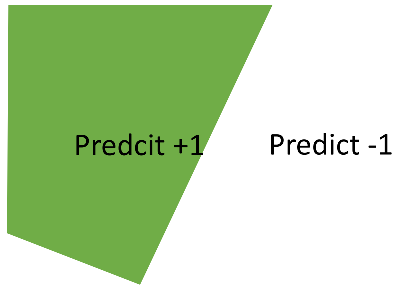
Positive Rays



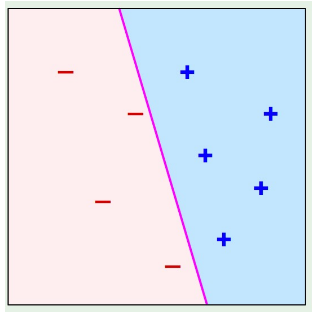
Positive Intervals



Convex Sets



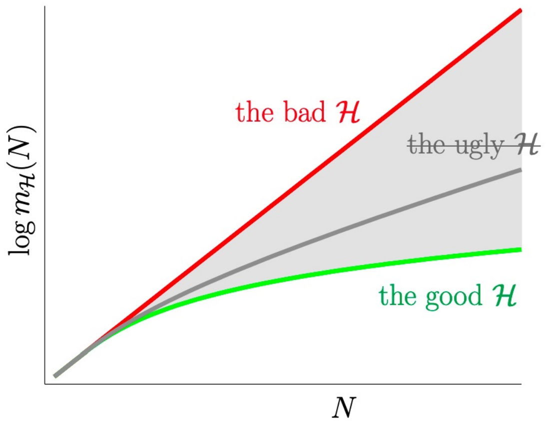
2D Perceptron



Bounding Growth Functions using Break Points

- Theorem statement:
  - If there is no break point for H, then $m_H(N) = 2^N$ for all N.
  - If k is a break point for H, i.e., if $m_H(k) < 2^k$ for some value k,

$$m_H(N) \leq \sum_{i=0}^{k-1} \binom{N}{i}$$



- Rephrase the 2nd point of the above theorem
  - If k is a break point for H, the following statements are true
    - $m_H(N) \leq N^{k-1} + 1$ [Can be proven using induction from above. See LFD Problem 2.5]
    - $m_H(N) = O(N^{k-1})$
    - $m_H(N)$ is polynomial in N
  - If d_{vc} is the VC dimension of H, then
    - $m_H(N) \leq \sum_{i=0}^{d_{vc}} \binom{N}{i}$
    - $m_H(N) \leq N^{d_{vc}} + 1$
    - $m_H(N) = O(N^{d_{vc}})$

If d_{vc} is the VC dimension of H, $d_{vc} + 1$ is a break point for H

Vapnik–Chervonenkis (VC) Bound

- VC Generalization Bound

  With prob at least $1 - \delta$

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4m_H(2N)}{\delta}}$$

- Let d_{vc} be the VC dimension of H, we have $\boldsymbol{m_H(N) \leq N^{d_{vc}} + 1}$. Therefore,

  With prob at least $1 - \delta$

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4((2N)^{d_{vc}}+1)}{\delta}}$$

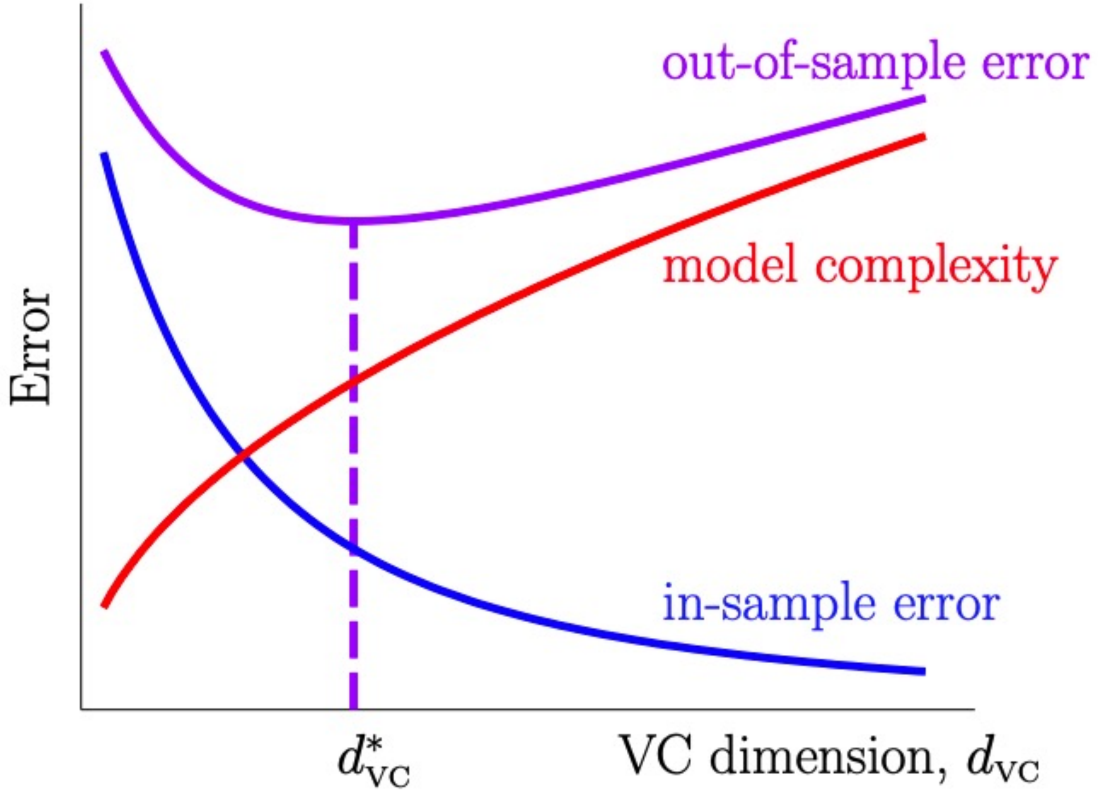
- If we treat δ as a constant, then we can say, with high probability

$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{vc} \frac{\ln N}{N}}\right)$$

Approximation-Generalization Tradeoff

- VC Dimension: A single parameter to characterize the complexity of H

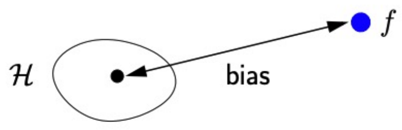
$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{vc}\frac{\ln N}{N}}\right)$$



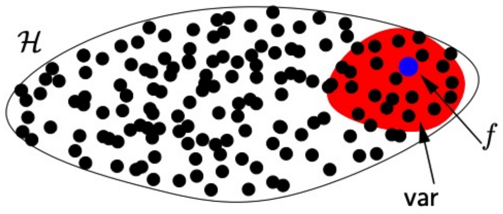
Bias-Variance Decomposition

- $$\mathbb{E}_D\left[E_{out}\left(g^{(D)}\right)\right] = \mathbb{E}_{\vec{x}}\left[\overset{\text{Bias}(\vec{x})}{\left(\bar{g}(\vec{x}) - f(\vec{x})\right)^2}\right] + \mathbb{E}_{\vec{x}}\left[\overset{\text{Var}(\vec{x})}{\mathbb{E}_D\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)^2\right]}\right]$$

- The performance of your learning, i.e., $\mathbb{E}_D\left[E_{out}\left(g^{(D)}\right)\right]$, depends on
  - How well you can fit your data using your hypothesis set (bias)
  - How close to the best fit you can get for a given dataset (variance)

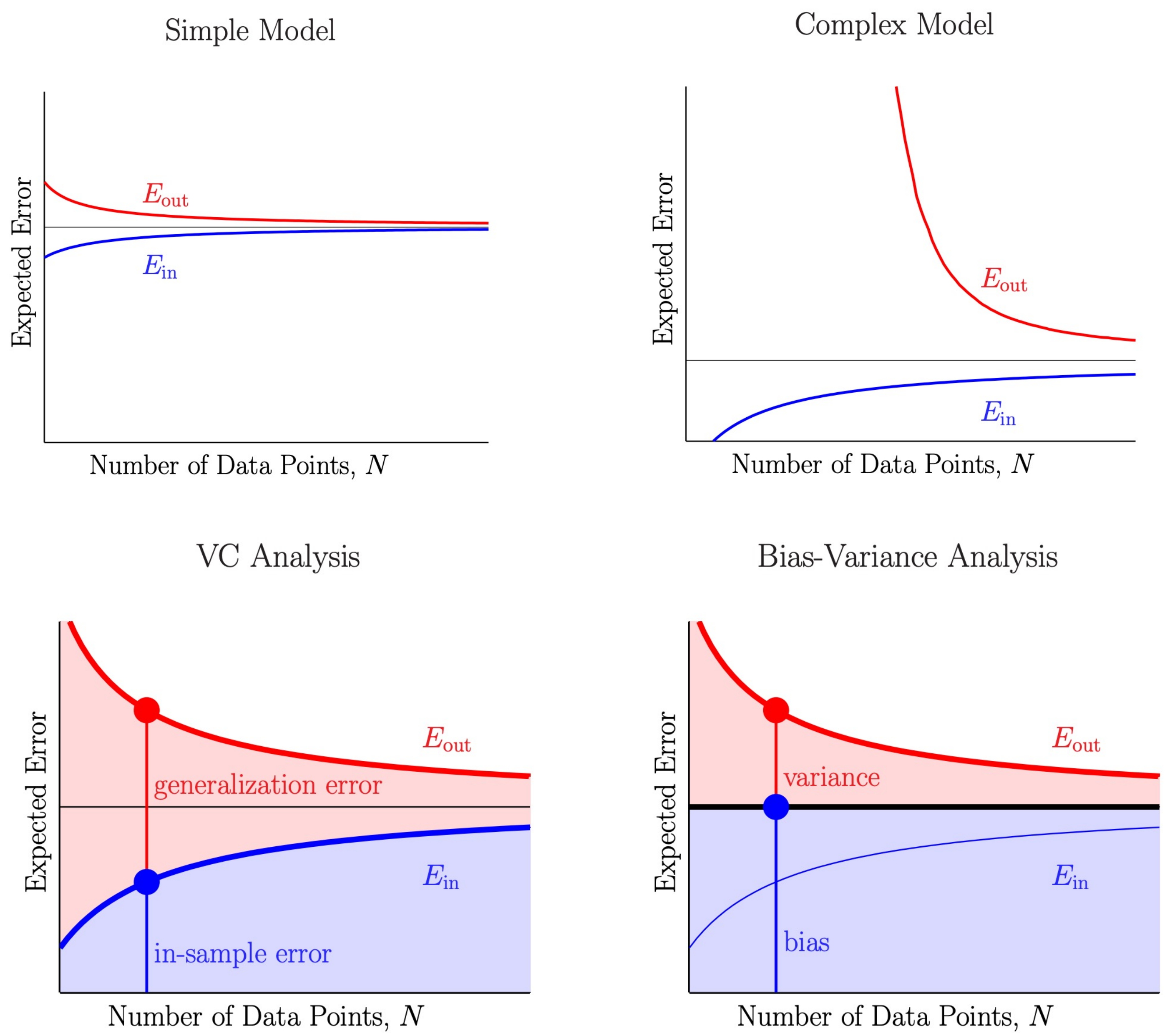


Very small model



Very large model

Learning Curves



Linear Models

This is why it's called linear models

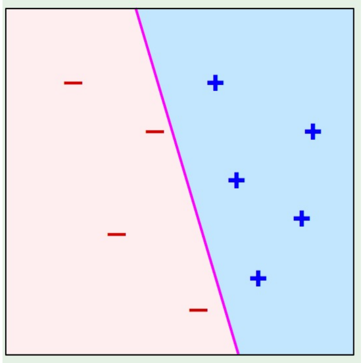
- H contains hypothesis $h(\vec{x})$ as **some function of $\vec{w}^T\vec{x}$**

	Domain	Model
Linear Classification	$y \in \{-1, +1\}$	$H = \{h(\vec{x}) = sign(\vec{w}^T\vec{x})\}$
Linear Regression	$y \in \mathbb{R}$	$H = \{h(\vec{x}) = \vec{w}^T\vec{x}\}$
Logistic Regression	$y \in [0,1]$	$H = \{h(\vec{x}) = \theta(\vec{w}^T\vec{x})\}$

$$\theta(s) = \frac{e^s}{1+e^s}$$

- Algorithm:
  - Focus on $g = argmin_{h \in H} E_{in}(h)$

Linear Classification

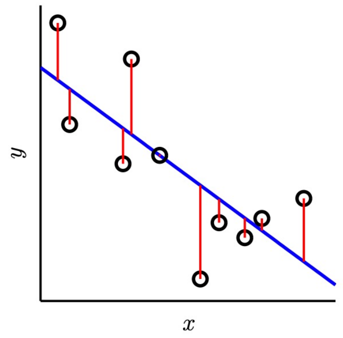


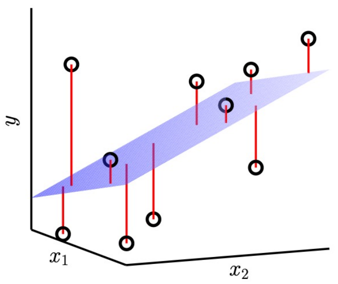
- Formulation
  - Hypothesis set $H = \{h(\vec{x}) = sign(\vec{w}^T \vec{x})\}$
  - Error measure: binary error $e(h(\vec{x}), y) = \mathbb{I}[h(\vec{x}) \neq y]$
- Data is linearly separable
  - Run PLA => $E_{in} = 0$ => Low E_{out}
- Data is not linearly separable
  - Engineering the features
  - Pocket algorithm

<u>Perceptron Learning Algorithm (PLA)</u>

Initialize $\vec{w}(0) = \vec{0}$
For $t = 0, \ldots$
  Find a misclassified example $(\vec{x}(t), y(t))$ in D
    that is, $\mathrm{sign}(\vec{w}(t)^T \vec{x}(t)) \neq y(t)$
  If no such sample exists
    Return $\vec{w}(t)$
  Else
    $\vec{w}(t+1) \leftarrow \vec{w}(t) + y(t)\vec{x}(t)$

Linear Regression

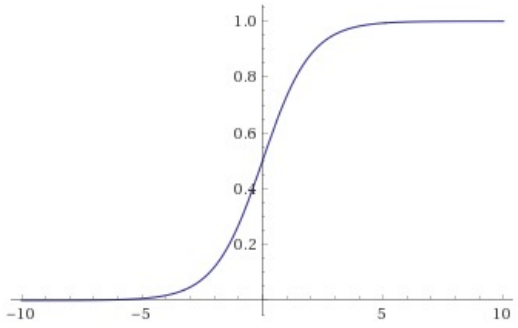




- Formulation
  - Hypothesis set $H = \{h(\vec{x}) = \vec{w}^T\vec{x}\}$
  - Squared error $e(h(\vec{x}), y) = (h(\vec{x}) - y)^2$

- Linear regression algorithm (one-step learning for solving $\nabla_{\vec{w}} E_{in}(\vec{w}_{lin}) = 0$)
  - Given $D = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_N, y_N)\}$
  - Construct $X = \begin{bmatrix} \vec{x}_1^T \\ \vdots \\ \vec{x}_N^T \end{bmatrix} = \begin{bmatrix} x_{1,0} & x_{1,1} & \cdots & x_{1,d} \\ x_{2,0} & x_{2,1} & \cdots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{2,0} & x_{N,1} & \cdots & x_{N,d} \end{bmatrix}$ and $\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$
  - Output $\vec{w}_{lin} = (X^T X)^{-1} X^T \vec{y}$ (Assume $X^T X$ is invertible)

Logistic Regression



- Hypothesis set $H = \{h(\vec{x}) = \theta(\vec{w}^T \vec{x})\}$
  - $\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}$
- Predict a probability
  - Interpreting $h(\vec{x})$ as the prob for $y = +1$ given $\vec{x}$ when h is the target function
- Algorithm
  - Find $g = argmin_{h \in H} E_{in}(h)$
- Two key questions
  - How to define $E_{in}(h)$?
  - How to perform the optimization (minimizing E_{in})?

Define $E_{in}(\vec{w})$: Cross-Entropy Error

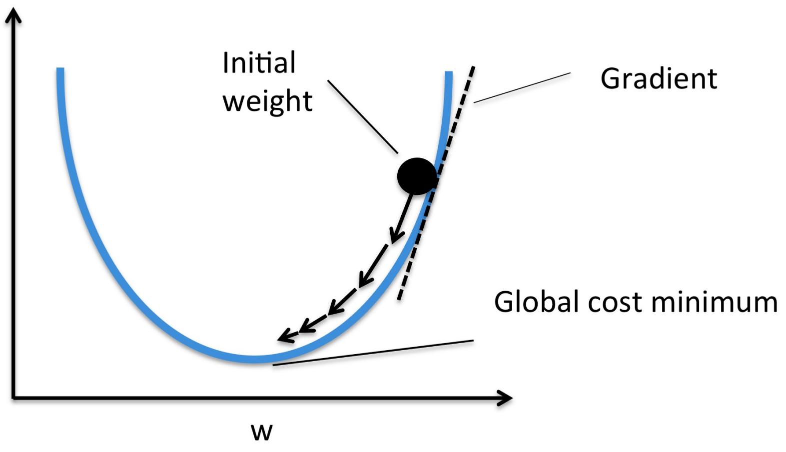
$$E_{in}(\vec{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$$

- Minimizing cross entropy error is the same as maximizing likelihood

- Likelihood: $\Pr(D|\vec{w})$
  - $\vec{w}^* = argmax_{\vec{w}} \Pr(D|\vec{w})$ (maximizing likelihood)
    $= argmin_{\vec{w}} E_{in}(\vec{w})$ (minimizing cross-entropy error)

Optimizing $E_{in}(\vec{w})$: Gradient Descent

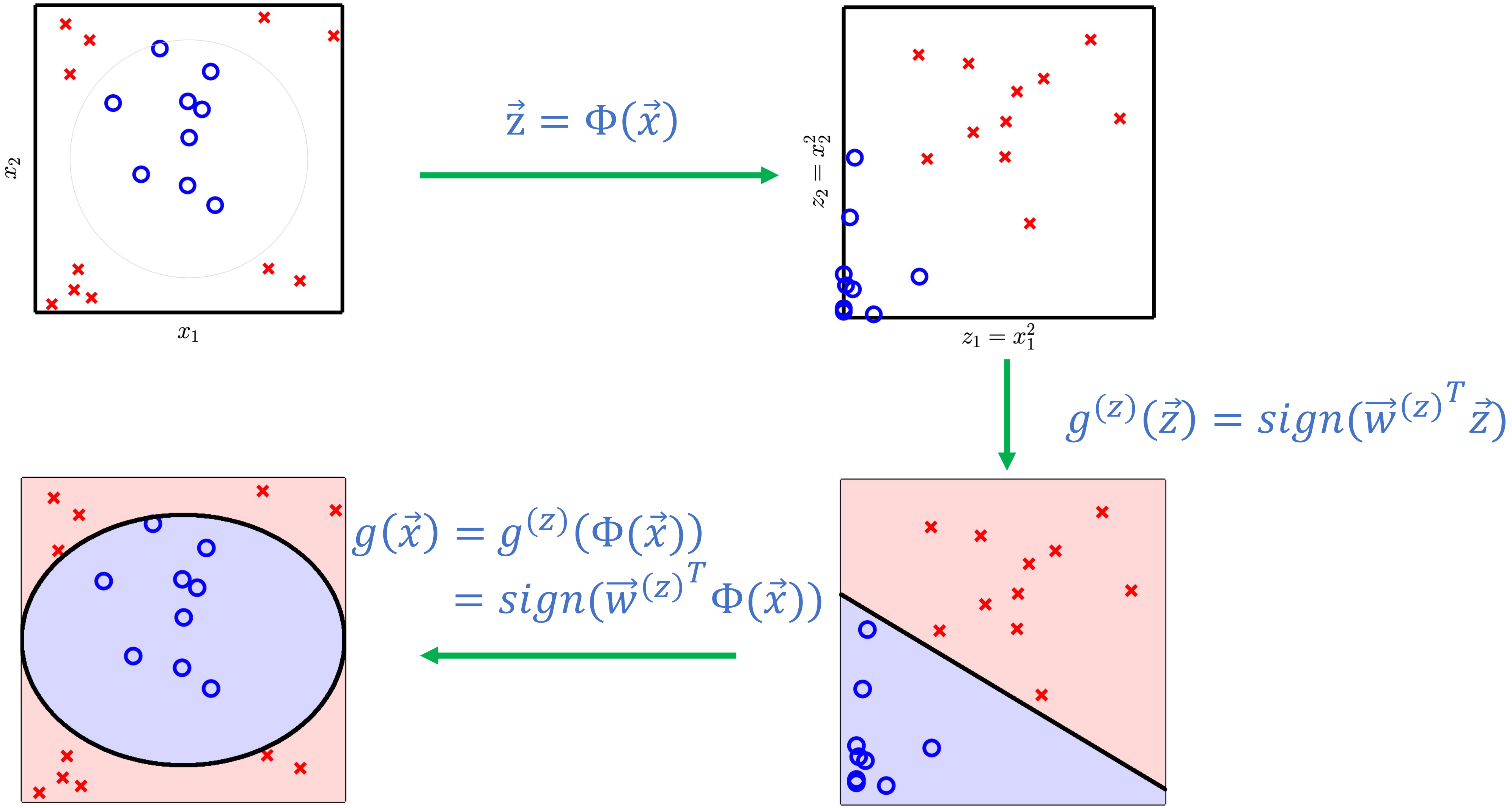
- Gradient descent algorithm
  - Initialize $\vec{w}(0)$
  - For $t = 0, \ldots$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}\big(\vec{w}(t)\big)$
    - Terminate if the stop conditions are met
  - Return the final weights



Works for functions where gradient exists everywhere

- Stochastic gradient decent
  - Replace the update step:
    - Randomly choose n from $\{1, \ldots, N\}$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} e_n(\vec{w}(t))$

Nonlinear Transformation



Must Choose Φ BEFORE Looking at the Data

- Rely on domain knowledge (feature engineering)
  - Handwriting digit recognition example

- Use common sets of feature transformation
  - Polynomial transformation
  - E.g., 2nd order Polynomial transformation
    - $\vec{x} = (1, x_1, x_2),\ \Phi_2(\vec{x}) = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$
    - Plus: more powerful (contains circle, ellipse, hyperbola, etc)
    - Minus:
      - More computation/storage
      - Worse generalization error

The VC dimension of d-dim perceptron is d+1

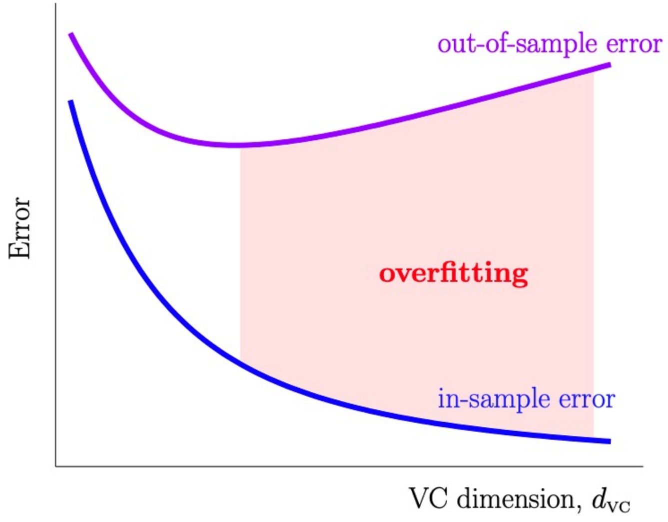
Q-th Order Polynomial Transform

- $\vec{x} = (1, x_1, \ldots, x_d)$
- $\Phi_1(\vec{x}) = \vec{x}$
- $\Phi_Q(\vec{x}) = (\Phi_{Q-1}(\vec{x}), x_1^Q, x_1^{Q-1} x_2, \ldots, x_d^Q)$

- Each element in $\Phi_Q(\vec{x})$ is in the form of $\sum_{i=1}^{d} x_i^{a_i}$
  - where $\sum_{i=1}^{d} a_i \leq Q$, and a_i is a non-negative integer

Overfitting and Its Cures

- Overfitting
  - Fitting the data more than is warranted
  - Fitting the noise instead of the pattern of the data
  - Decreasing E_{in} but getting larger E_{out}
  - When H is too strong, but N is not large enough



- Regularization
  - Intuition: Constraining H to make overfitting less likely to happen
- Validation
  - Intuition: Reserve data to estimate E_{out}

Regularization

- Constrain H
  - Example: Weight decay $H(C) = \{h \in H_Q \text{ and } \vec{w}^T\vec{w} \leq C\}$
  - Finding g => Constrained optimization

minimize $E_{in}(\vec{w})$

subject to $\vec{w}^T\vec{w} \leq C$

- Define augmented error
  - $E_{aug}(h, \lambda, \Omega) = E_{in}(\vec{w}) + \frac{\lambda}{N}\Omega(h)$
  - Finding g => Unconstrained optimization

minimize $E_{in}(\vec{w}) + \frac{\lambda_C}{N}\vec{w}^T\vec{w}$

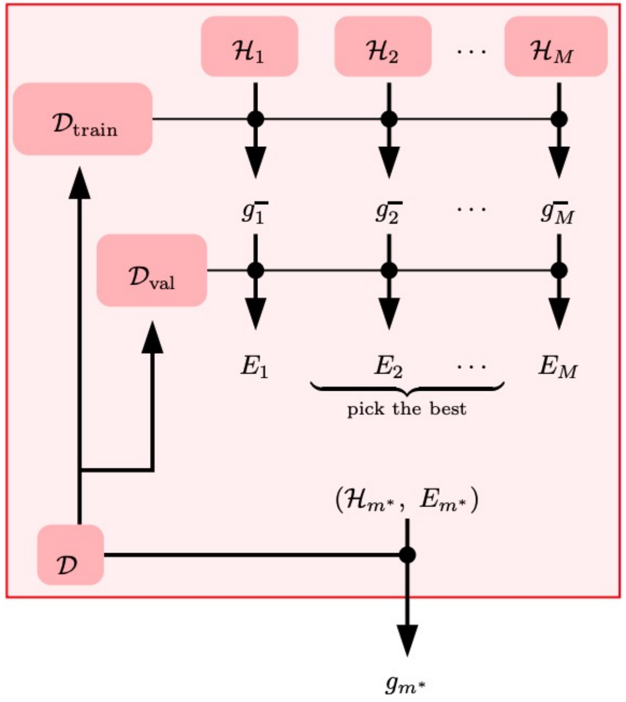
- The two interpretations are conceptually equivalent in a lot of cases.

- **Understand the impacts of choosing $\boldsymbol{\Omega}$ and $\boldsymbol{\lambda}$**

Validations

- Reserving data to estimate E_{out}

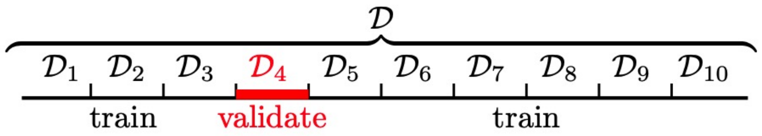
Model Selection



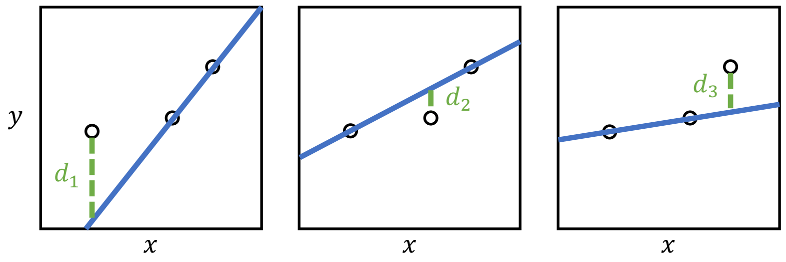
	Outlook	Relationship to E_{out}
E_{in}	Incredibly optimistic	VC-bound
E_{val} (when used for model selection)	Slightly optimistic	Hoeffding's bound (multiple hypotheses)
E_{test}	Unbiased	Hoeffding's bound (single hypothesis)

Cross Validation

- Split D into V equally sized data sets: $D_1, D_2, \ldots, D_V$
  - Let g_i^- be the hypothesis learned using all data sets except D_i
  - Let $e_i = E_{val}(g_i^-)$ where the validation uses data set D_i
- The V-fold cross validation error is $\frac{1}{V}\sum_{i=1}^{V} e_i$



- Leave-One-Out Cross Validation (LOOCV): $V = N$



$$E_{cv} = \frac{1}{3}(d_1^2 + d_2^2 + d_3^2)$$

Three Learning Principles

- Occam's Razor
  - The simplest model that fits the data is also the most plausible
- Sampling Bias
  - If the data is sampled in a biased way, learning will produce a similarly biased outcome.
- Data Snooping
  - If a data set has affected any step in the learning process, its ability to assess the outcome has been compromised.

Practice Questions

Don’t view these as good representations of exam questions.

But it should give you a sense of what the exam questions might look like.