COMP5211: Machine Learning

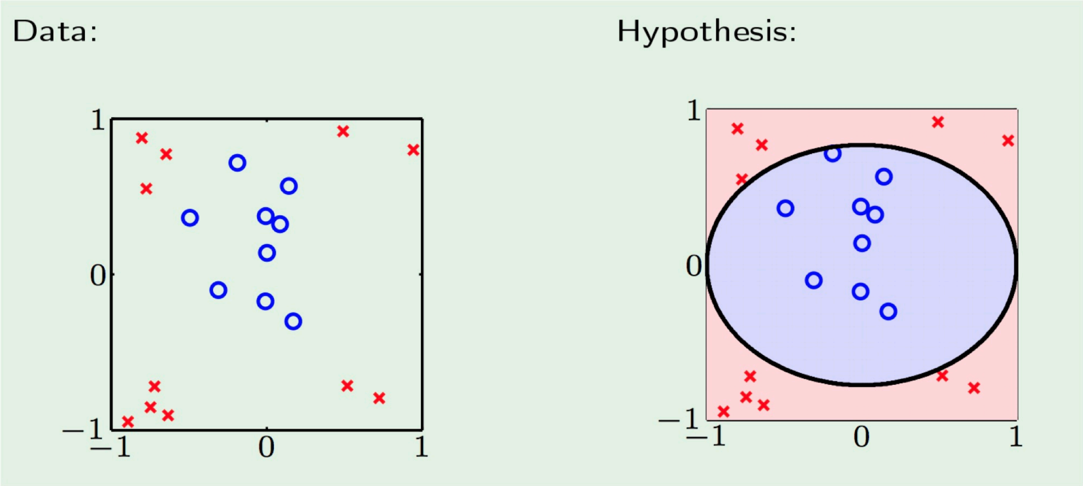
Lecture 7

Minhao Cheng

From last lecture

Linear hypotheses

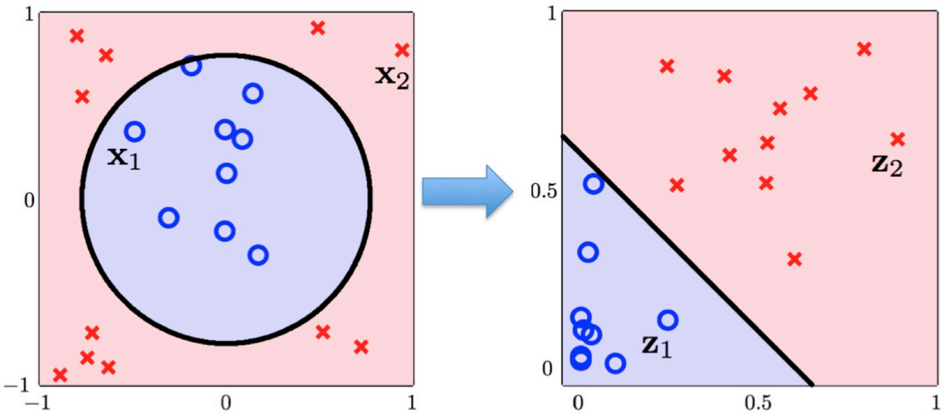
- Up to now: linear hypotheses
  - Perception, Linear regression, Logistic regression, …
- Many problems are not linearly separable



Nonlinear transformation

Circular Separable and Linear Separable

- $$h(x) = \text{sign}(\underbrace{0.6}_{\tilde{w}_0} \cdot \underbrace{1}_{\tilde{z}_0} + \underbrace{(-1)}_{\tilde{w}_1} \cdot \underbrace{x_1^2}_{\tilde{z}_1} + \underbrace{(-1)}_{\tilde{w}_2} \cdot \underbrace{x_2^2}_{\tilde{z}_2})$$
  $$= \text{sign}(\tilde{w}^T z)$$
- $\{(x_n, y_n)\}$ circular separable $\Rightarrow$ $\{(z_n, y_n)\}$ linear separable
- $x \in \mathcal{X} \rightarrow x \in \mathcal{Z}$ (using a nonlinear transformation ϕ)



Nonlinear Transformation

Definition

- Define nonlinear transformation
  - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$
- Linear hypotheses in $\mathcal{Z}$-space:
  - $\text{sign}(\tilde{h}(\mathbf{z})) = \text{sign}(\tilde{h}(\phi(\mathbf{x}))) = \text{sign}(w^T \phi(\mathbf{x}))$
- Line in $\mathcal{Z}$-space $\Leftrightarrow$ some quadratic curves in $\mathcal{X}$-space

Nonlinear Transformation

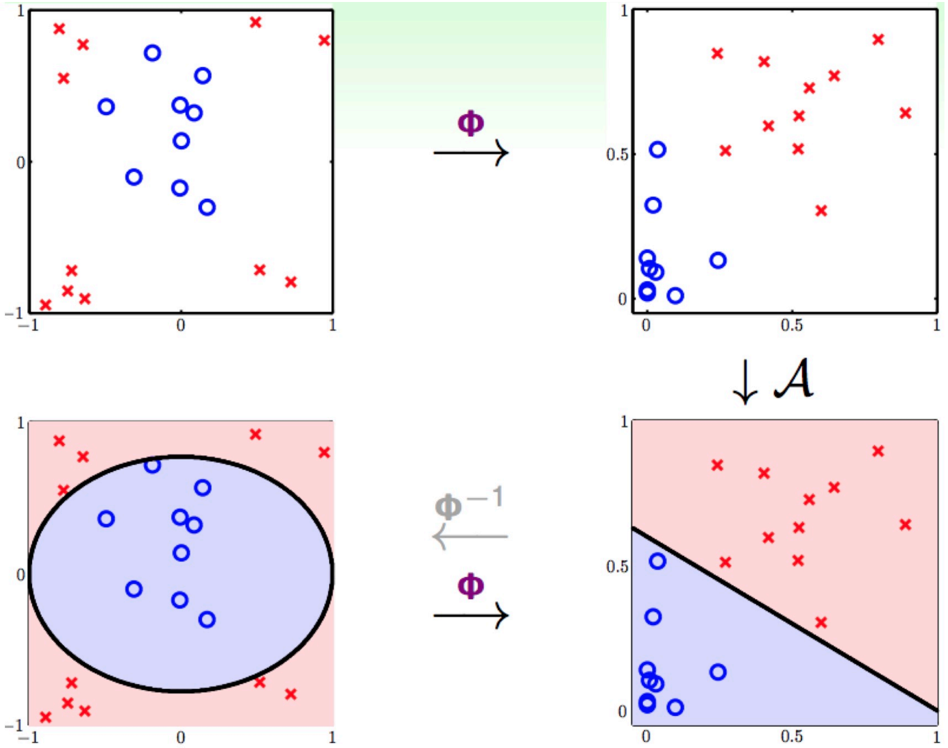
General Quadratic Hypothesis Set

- A “bigger ” $\mathscr{Z}$-space:
  - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$
- Linear in $\mathscr{Z}$-space ⇔ quadratic hypotheses in $\mathscr{X}$-space
- The hypotheses space:
  - $\mathscr{H}_{\phi_2} = \{h(x) : h(x) = \tilde{w}^T \phi_2(x)$ for some $\tilde{w}\}$ (quadratic hypotheses)
- Also include linear model as a degenerate case

Nonlinear transformation

Learning a good quadratic function

- Transform original data $\{x_n, y_n\}$ to $\{z_n = \phi(x_n), y_n\}$
- Solve a linear problem on $\{z_n, y_n\}$ using your favorite algorithm $\mathscr{A}$ to get a good model $\tilde{w}$
- Return the model $h(x) = \text{sign}(\tilde{w}^T \phi(x))$



Nonlinear transformation

Polynomial mappings

- Can now freely do quadratic classification, quadratic regression
- Can easily extend to any degree of polynomial mappings
  - E.g.,
    $\phi(x) = (x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2^2, x_1x_3^2, x_1x_2^2, x_2^2x_3, x_2^2x_3, x_1^3, x_2^3, x_3^3)$

Nonlinear Transformation

The price we pay: computational complexity

- Q-th oder polynomial transform:

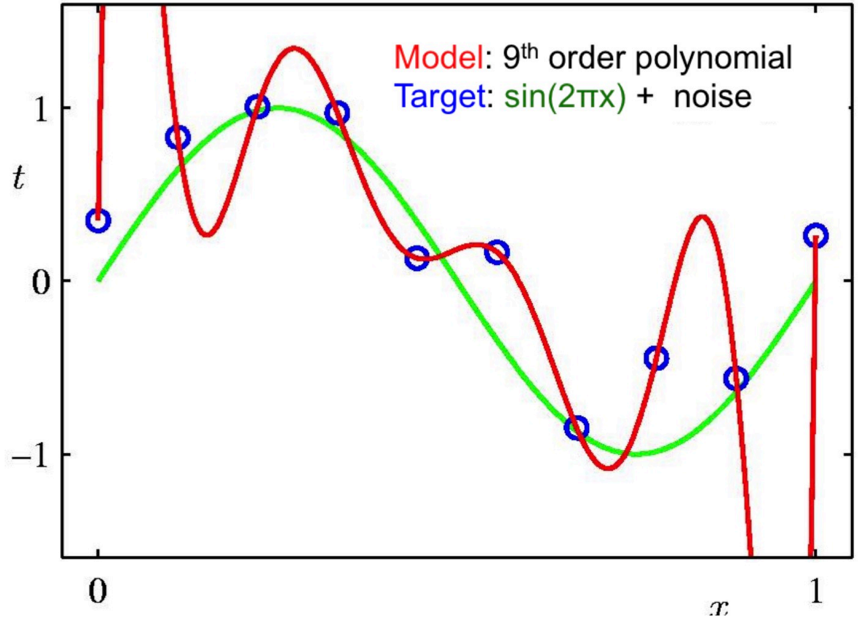
$$\phi(x) = (1, x_1, x_2, \ldots, x_d,$$
$$x_1^2, x_1 x_2, \ldots, x_d^2, \ldots, x_d^2,$$
$$\cdots$$
$$x_1^Q, x_1^{Q-1} x_2, \ldots, x_d^Q)$$

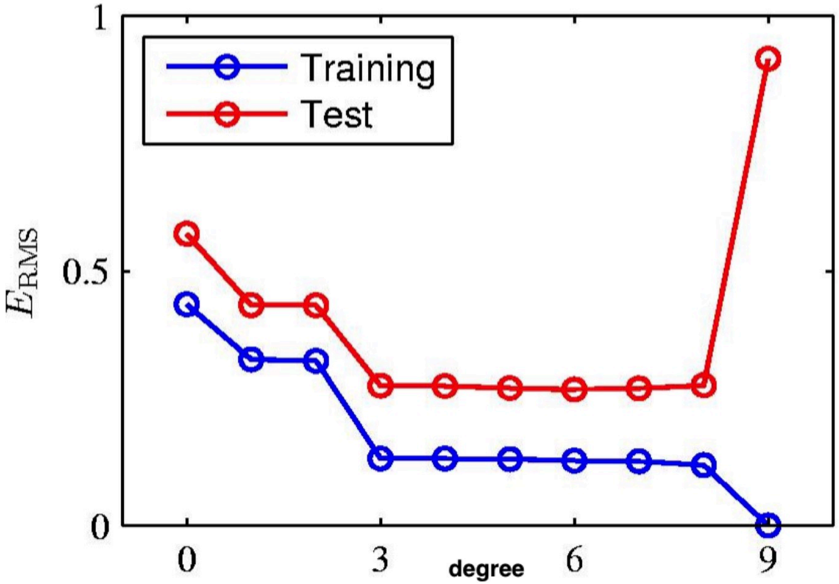
- $O(d^Q)$ dimensional vector $\Rightarrow$ High computational cost
  - Kernel method

Nonlinear Transformation

The price we pay: overfitting

- Overfitting: the model has low training error but high prediction error





Theory of Generalization

Training versus testing

- Machine learning pipeline:
  - Training phase:
    - Obtain the best model h by minimizing training error
  - Test (inference) phase:
    - For any incoming test data x”
      - Make prediction by $h(x)$
    - Measure the performance of h: test error

Theory of Generalization

Training versus testing

- Does low training error imply low test error?
  - They can be totally different if
    - train distribution $\neq$ test distribution

Theory of Generalization

Training versus testing

- Does low training error imply low test error?
  - They can be totally different if
    - train distribution $\neq$ test distribution
  - Even under the same distribution, they can be very different:
    - Because h is picked to minimize training error, not test error

Theory of Generalization

Formal definition

- Assume training and test data are both sampled from D
- The ideal function (for generating labels) is $f : f(x) \rightarrow y$
- Training error: Sample $x_1, \ldots, x_N$ from D and
    - $E_{tr}(h) = \frac{1}{N}\sum_{n=1}^{N} e(h(x_n), f(x_n))$
    - h is determined by $x_1, \ldots, x_n$
- Test error: Sample $x_1, \ldots, x_N$ from D and
    - $E_{te}(h) = \frac{1}{M}\sum_{m=1}^{M} e(h(x_m), f(x_m))$
    - h is independent to $x_1, \ldots, x_n$

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  - h is independent to $x_1, \ldots, x_n$
- Generalization error = Test error = Expected performance on D:
  - $E(h) = \mathbb{E}_{x \sim D}[e(h(x), f(x))] = E_{te}(h)$

Theory of Generalization

The 2 questions of learning

- $E(h) \approx 0$ is achieved through:
  - $E(h) \approx E_{tr}(h)$ and $E_{tr}(h) \approx 0$

Theory of Generalization

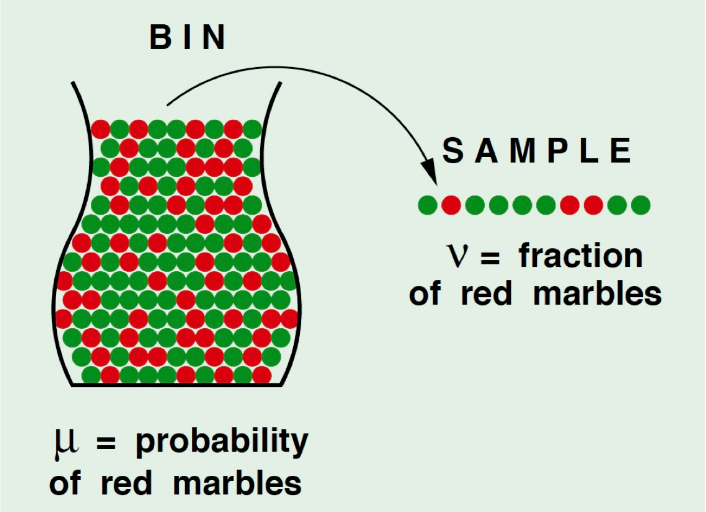
The 2 questions of learning

- $E(h) \approx 0$ is achieved through:
  - $E(h) \approx E_{tr}(h)$ and $E_{tr}(h) \approx 0$
- Learning is split into 2 questions:
  - Can we make sure that $E(h) \approx E_{tr}(h)$?
    - Today's focus
  - Can we make $E_{tr}(h)$ small?
    - Optimization

Theory of Generalization

Bound $\|E(h) - E_{tr}(h)\|$

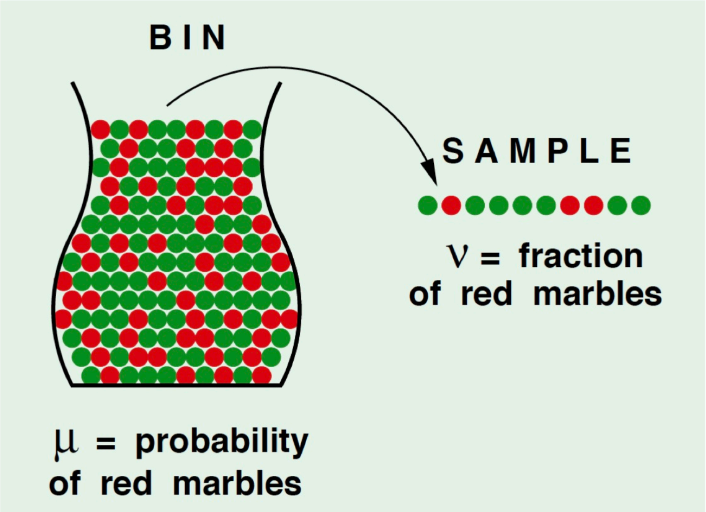
- Consider a bin with red and green marbles
    - P[picking a red mable] $= \mu$
    - P[picking a green mable] $= 1 - \mu$
- The value of μ is unknown to us
- How to infer μ?
    - Pick N marbles independently
    - ν: the traction of red marble



Theory of Generalization

Inferring with probability

- Do we **know** μ
  - No
  - Sample can be mostly green while bin is mostly red
- Can we say something about μ?
  - Yes
  - ν is "probably" close to μ



Theory of Generalization

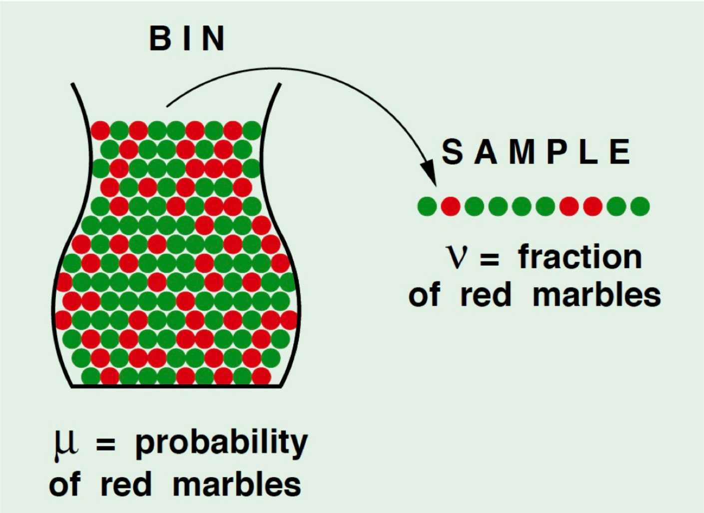
Hoeffding's inequality

- In big sample (large N), ν (sample mean) is probably close to μ:
    - $p[\,|\nu - \mu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
    - This is called **Hoeffding's inequality**
- The statement "$\mu = \nu$" Is probably approximately correct (PAC)

Theory of Generalization

Hoeffding's inequality

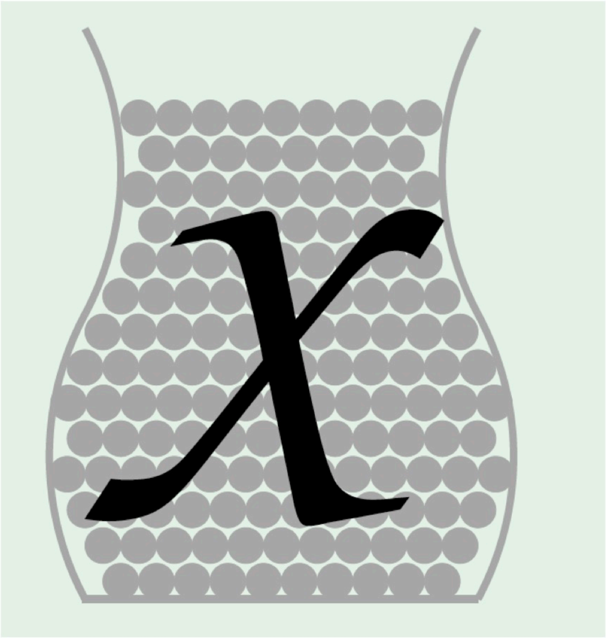
- $p[\,|\nu - \mu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
  - Valid for all N and $\epsilon > 0$
  - Does not depend on μ (no need to know μ)
  - Larger sample size N or looser gap $\epsilon \Rightarrow$ higher probability for $\mu \approx \nu$



Theory of Generalization

Connection to Learning

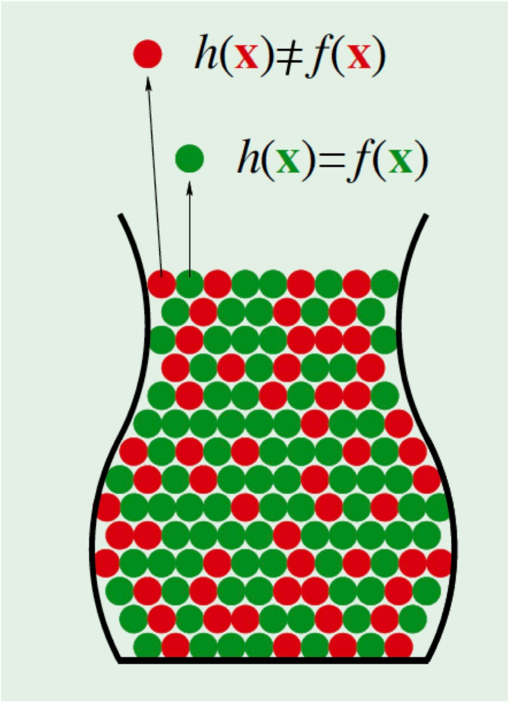
- How to connect this to learning?
  - Each marble (uncolored) is a data point $x \in \mathcal{X}$



Theory of Generalization

Connection to Learning

- How to connect this to learning?
  - Each marble (uncolored) is a data point $x \in \mathcal{X}$
  - Red marble: $h(x) \neq f(x)$
  - Green marble: $h(x) = f(x)$



Theory of Generalization

Connection to Learning

- Given a function h
- If we randomly draw $x_1, \ldots, x_n$ (independent to h):
  - $E(h) = \mathbb{E}_{x \sim D}[h(x) \neq f(x)] \Leftrightarrow \mu$ (generalization error, unknown)
  - $\frac{1}{N} \sum_{n=1}^{N} [h(x_n) \neq y_n] \Leftrightarrow \nu$ (error on sampled data, known)

Theory of Generalization
Connection to Learning

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- Based on Hoeffding's inequality:
    - $p[\,|\nu - \mu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
- "$\mu = \nu$" Is probably approximately correct (PAC)

Theory of Generalization

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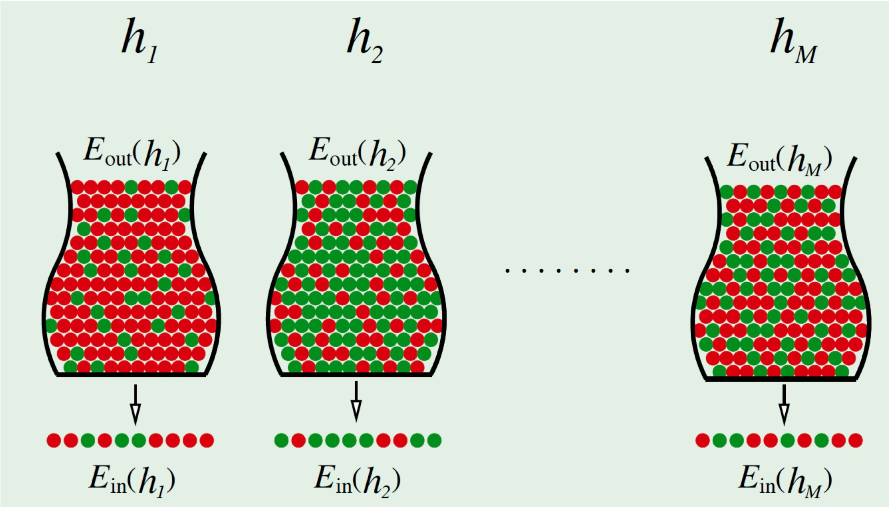
- Based on Hoeffding's inequality:
  - $p[\,|\nu - \mu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
- "$\mu = \nu$" Is probably approximately correct (PAC)
- However, this can only "verify" the error of a hypothesis:
  - h and $x_1, \ldots, x_N$ must be independent

Theory of Generalization

Apply to multiple bins (hypothesis)

- Can we apply to multiple hypothesis?
- Color in each bin depends on different hypothesis
  - Bingo when getting all green balls?



Theory of Generalization

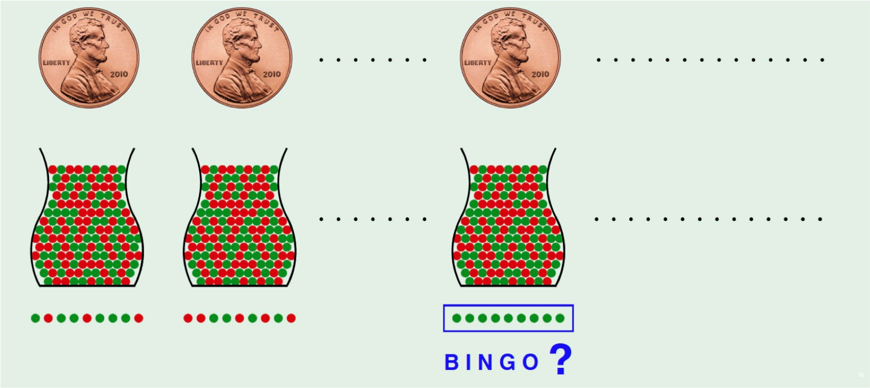
Coin game

- If you have 150 **fair** coins, flip each coin 5 times, and one of them gets 5 heads. Is this coin (g) special?

- No. The probability of exiting at least one of the coin results in 5 heads is

$$1 - (\frac{31}{32})^{150} > 99\,\%$$

- Because: there can exist some h such that E and E_{tr} are far way if M is large.



M -> number of hypothesis

Theory of Generalization

A simple solution

- For each particular h,
  - $P[\,|E_{tr}(h) - E(h)| > \epsilon] \leq 2e^{-2\epsilon^2 N}$
- If we have a hypothesis set $\mathscr{H}$,we want to derive the bound for $P[\sup_{h\in\mathscr{H}}|E_{tr}(h) - E(h)| > \epsilon]$
  - $P[\,|E_{tr}(h_1) - E(h_1)| > \epsilon]$ or … or $P[\,|E_{tr}(h_{|\mathscr{H}|}) - E(h_{|\mathscr{H}|})| > \epsilon]$
  - $\leq \sum_{m=1}^{\mathscr{H}} P[\,|E_{tr}(h_m) - E(h_m)|\,] \leq 2|\mathscr{H}|e^{-2\epsilon^2 N}$
    - Because of union bound inequality $P(\bigcup_{i=1}^{\infty} A_i) \leq \sum_{i=1}^{\infty} P(A_i)$

Theory of generalization

When is learning successful?

- When our learning algorithm $\mathscr{A}$ picks the hypothesis g:
  - $P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E(h) | > \epsilon] \leq 2 | \mathscr{H} | e^{-2\epsilon^2 N}$
- If $| \mathscr{H} |$ is small and N is large enough:
  - If $\mathscr{A}$ finds $E_{tr}(g) \approx 0 \Rightarrow E(g) \approx 0$ (Learning is successful!)

Theory of Generalization

Feasibility of Learning

- $P[\,|E_{tr}(g) - E(g)| > \epsilon] \leq 2\,|\mathcal{H}|\,e^{-2\epsilon^2 N}$
  - Two questions:
    - 1. Can we make sure $E(g) \approx E_{tr}(g)$?
    - 2. Can we make sure $E_{tr}(g) \approx 0$?

Theory of Generalization

Feasibility of Learning

- $P[\,|E_{tr}(g) - E(g)| > \epsilon] \leq 2|\mathcal{H}|e^{-2\epsilon^2 N}$
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- $|\mathcal{H}|$: complexity of model
  - Small $|\mathcal{H}|$: 1 holds, but 2 may not hold (too few choices) (under-fitting)

Theory of Generalization

Feasibility of Learning

- $P[\,|E_{tr}(g) - E(g)| > \epsilon] \leq 2\,|\mathcal{H}|\,e^{-2\epsilon^2 N}$
  - Two questions:
    - 1. Can we make sure $E(g) \approx E_{tr}(g)$?
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- $|\mathcal{H}|$: complexity of model
  - Small $|\mathcal{H}|$: 1 holds, but 2 may not hold (too few choices) (under-fitting)
  - Large $|\mathcal{H}|$: 1 doesn't hold, but 2 may hold (over-fitting)

Theory of Generalization

Feasibility of Learning

- Currently we only know
    - $P[\text{SUP}_{h\in\mathscr{H}}\,|\,E_{tr}(h) - E(h)\,| > \epsilon] \leq 2\,|\,\mathscr{H}\,|\,e^{-2\epsilon^2 N}$

Theory of Generalization

Feasibility of Learning

- Currently we only know
    - $P[\text{SUP}_{h \in \mathscr{H}} |E_{tr}(h) - E(h)| > \epsilon] \leq 2 |\mathscr{H}| e^{-2\epsilon^2 N}$
- What if $|\mathscr{H}| = \infty$?
    - (e.g. linear hyperplanes)

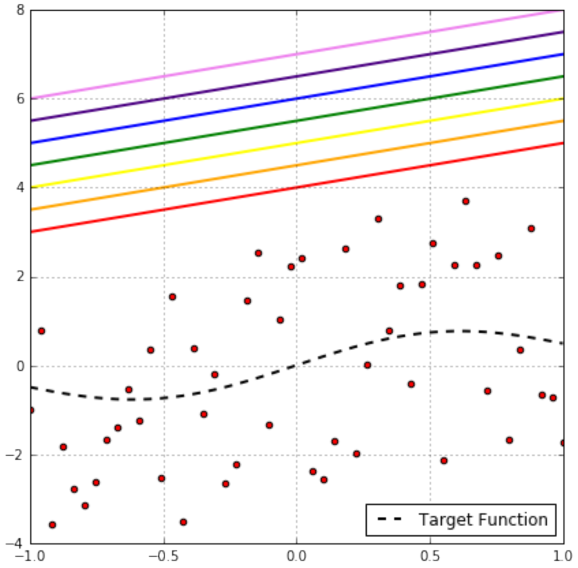
Theory of Generalization

Deduce the dimension

- Why do we need to consider every possible hypothesis?
  - $P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E(h) | > \epsilon]$
  - If we omit one hypothesis, we might miss the biggest gap
- $P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E(h) | > \epsilon] \leq 2 | \mathscr{H} | e^{-2\epsilon^2 N}$
  - from the union bound, which assume the event is independent

Theory of Generalization
Deduce the dimension

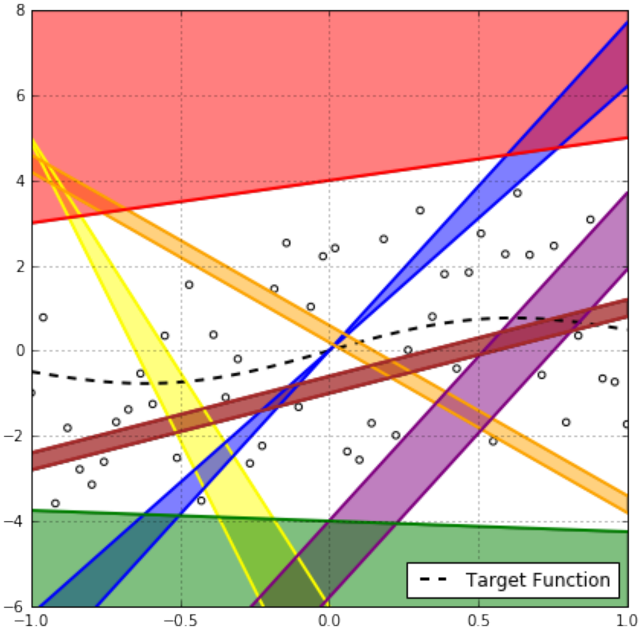
- Why do we need to consider every possible hypothesis?
    - $P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E(h) | > \epsilon]$
    - If we omit one hypothesis, we might miss the biggest gap
- However, are the events of each hypothesis having a big generalization gap are likely to be independent?



Theory of Generalization

Deduce the dimension

- Why do we need to consider every possible hypothesis?
    - $P[\textcolor{blue}{\mathrm{SUP}}_{h \in \mathscr{H}} |E_{tr}(h) - E(h)| > \epsilon]$
    - If we omit one hypothesis, we might miss the biggest gap
- However, are the events of each hypothesis having a big generalization gap are likely to be independent?
    - No



Theory of Generalization

Symmetrization lemma

- Imagine we have the ghost dataset S' with also size N:
- $P[\text{SUP}_{h \in \mathscr{H}} |E_{tr}(h) - E(h)| > \epsilon] \leq 2P[\text{SUP}_{h \in \mathscr{H}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$

Theory of Generalization

Growth function

- Imagine we have the ghost dataset S' with also size N:
  - $P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E(h) | > \epsilon] \leq 2P[\text{SUP}_{h \in \mathscr{H}} | E_{tr}(h) - E'_{tr}(h) | > \frac{\epsilon}{2}]$
- By union bound:
  - $P[\text{SUP}_{h \in \mathscr{H}_{S \cup S'}} | E_{tr}(h) - E'_{tr}(h) | > \frac{\epsilon}{2}] \leq | \mathscr{H}_{S \cup S'} | P[| E_{tr}(h) - E'_{tr}(h) | > \frac{\epsilon}{2}]$

Theory of Generalization

Growth function

- Imagine we have the ghost dataset S' with also size N:
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- By union bound:
  - $P[\text{SUP}_{h \in \mathcal{H}_{S \cup S'}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}] \leq |\mathcal{H}_{S \cup S'}| P[|E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$
- How to bound $|\mathcal{H}_{S \cup S'}|$

Theory of Generalization

Growth function

- For binary classification {+1,-1}, for a dataset with N samples,
  - The max number of distinct labellings is 2^N
- Growth function $\Delta_{\mathscr{H}}(N)$: The max number of distinct labellings on a dataset S of size N by a hypothesis space $\mathscr{H}$
- So,
  - $P[\mathrm{SUP}_{h \in \mathscr{H}_{S \cup S'}} |E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}] \leq \Delta_{\mathscr{H}}(2N) P[|E_{tr}(h) - E'_{tr}(h)| > \frac{\epsilon}{2}]$
  - And $\Delta_{\mathscr{H}}(N) \leq 2^m$