Learning Theory-Infinite Hypothesis sets

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Generalization bound (M hypotheses)

- Hoeffdeing's Inequality of the selected g hypothesis out of M hypotheses using N training points.

$$\boxed{\Pr[|Ein(g) - Eout(g)| > \varepsilon] \leq 2Me^{-2\varepsilon^2 N}}$$

Then, with probability at least 1-δ:

$$Eout(g) \leq Ein(g) + \varepsilon$$

$$\boxed{Eout(g) \leq Ein(g) + \sqrt{\frac{1}{2N}\ln(\frac{2M}{\delta})}}$$

where $\delta = 2Me^{-2\varepsilon^2 N}$

Generalization bound

- What if we have an infinite set of hypotheses?
- Example: the perceptron learning algorithm.

- Can we derive a generalization bound?

Review: Union bound of M hypotheses

Remember that M comes from applying a union bound.

Let the bad events B_i be:

$\Pr[B_i] = \mathrm{P}[|Ein(h_i) - Eout(h_i)\,| > \varepsilon]$

The union bound for M hypotheses:

$\mathrm{P}[B_1\ or\ B_2 or \ldots or B_M] \leq \mathrm{P}[B_1]+ \mathrm{P}[B_2]+\ldots.\ \mathrm{P}[B_M] \leq \sum_{i=1}^{M} \Pr[B_i]$

M terms

Since P(|Ein(h_i)-Eout(h_i)|>ε)≤$2e^{-2\varepsilon^2 N}$

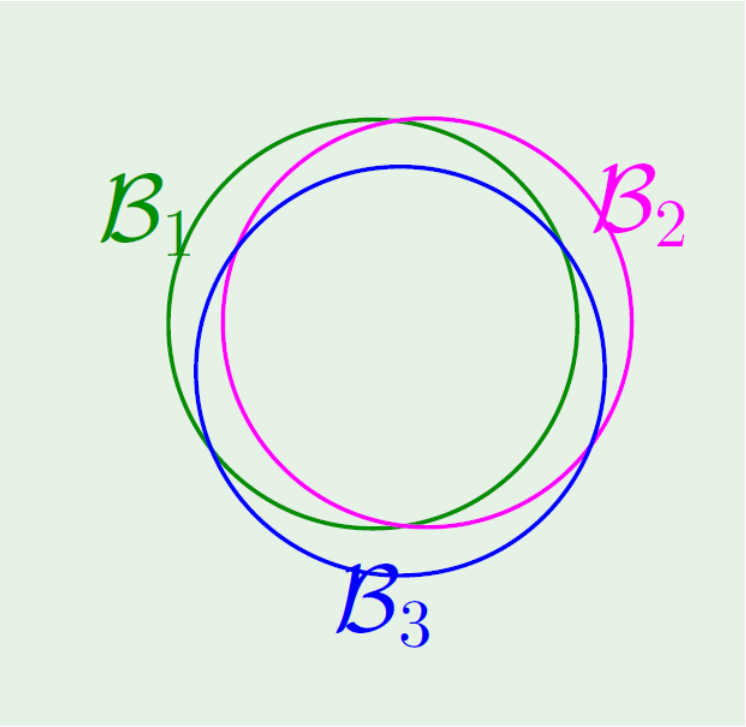
Then, P(|Ein(g)-Eout(g)|>ε)≤$2Me^{-2\varepsilon^2 N}$

Union bound of M hypotheses

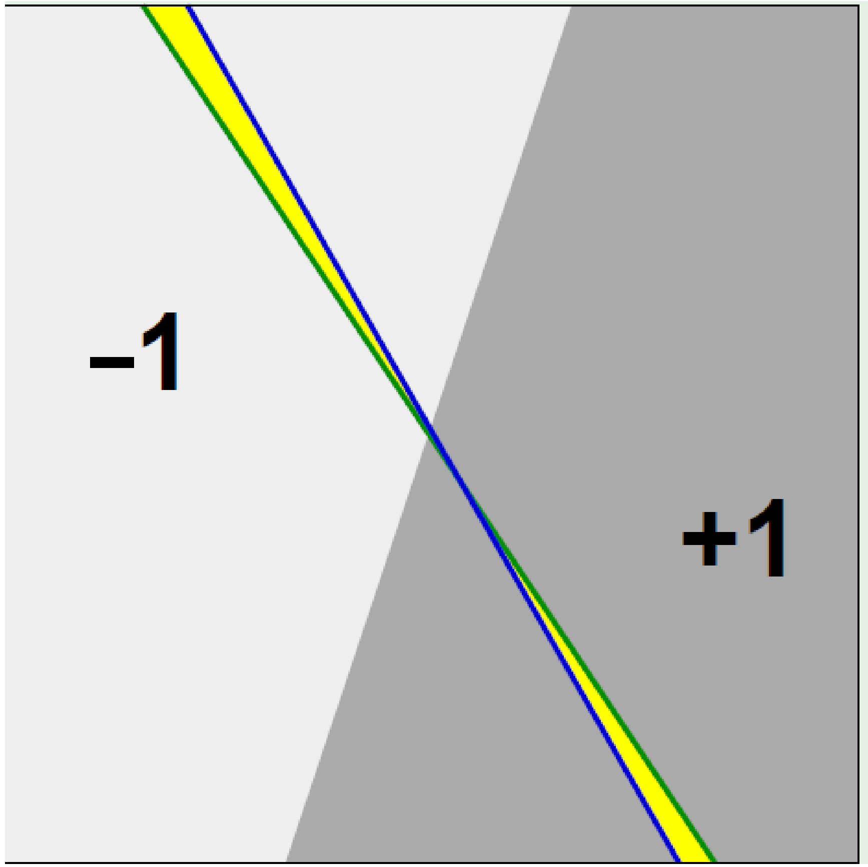
- The good news is that the B events are overlapping!!
- Since many hypotheses are similar, so their corresponding

B events $\mathrm{P}|Ein(h_i) - Eout(h_i)\ | > \varepsilon]$ are overlapping.

- Thus, the derived union bound was loose.
- We shall derive a tighter bound for infinite hypotheses.



Example- linear classifiers



Dichotomies

- For a binary classification problem:

A hypothesis h: X -> {+1,-1}.

- Apply a hypothesis h to a finite sample of input points not the whole input space.
- Assume we have N sample points $\{x_1, x_2, \ldots x_N\}$
- Apply h $\in$H to the N points, we get a dichotomy which is an N-tuple of $(h(x_1), h(x_2), \ldots h(x_N))$.

Dichotomies (cont.)

- For a hypothesis set H, the dichotomies generated by H are defined as:

$$H(x_1, x_2, \dots x_N) = \{(h(x_1), h(x_2), \dots h(x_N)) | h \in H\}$$

- A hypothesis h: X -> {+1,-1}.
- A dichotomy: $\{x_1, x_2, \dots x_N\} \to \{+1,-1\}$
- Number of hypotheses |H| can be infinite.
- Maximum number of dichotomies $|H(x_1, x_2, \dots x_N)|$ is 2^N.
- The greater the number of dichotomies $|H(x_1, x_2, \dots x_N)|$ is the more diverse and powerful the hypothesis set H.

Growth Function

- The growth function $m_H(N)$ for a hypothesis set H is defined as:
  - The largest number of dichotomies that can be generated by H on any N points.

$$m_H(N) = max_{x_1, x_2, \ldots, x_N \in X} |H(x_1, x_2, \ldots, x_N)|$$

- Since the maximum number of dichotomies $|H(x_1, x_2, \ldots x_N)|$ is 2^N, then:

$$m_H(N) \leq 2^N$$

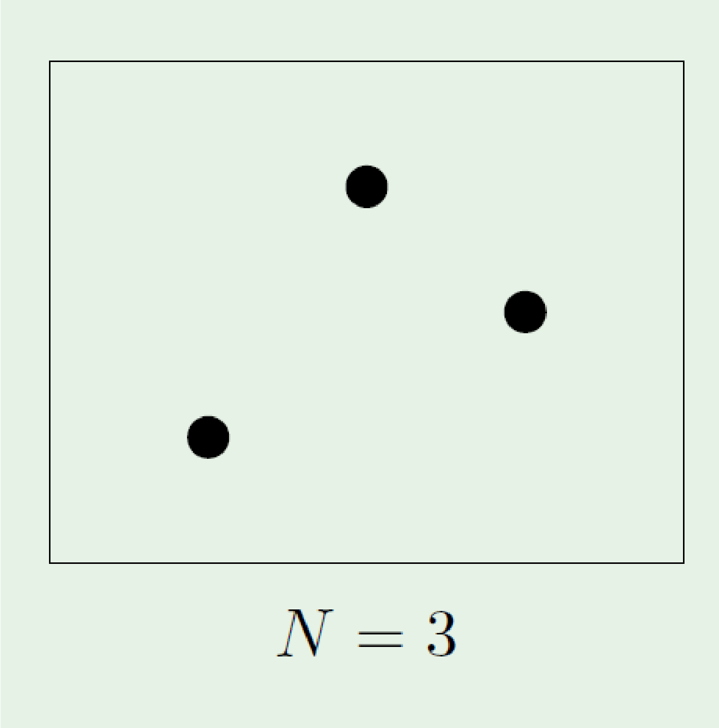
Growth Function (cont.)

- Given H, if H can generate all possible dichotomies on data points $(x_1, x_{2,\ldots} \, x_N)$ such that $|H(x_1, x_{2,\ldots} \, x_N)|=2^N$ then H shatters $(x_1, x_{2,\ldots} \, x_N)$.

Growth function-Perceptron

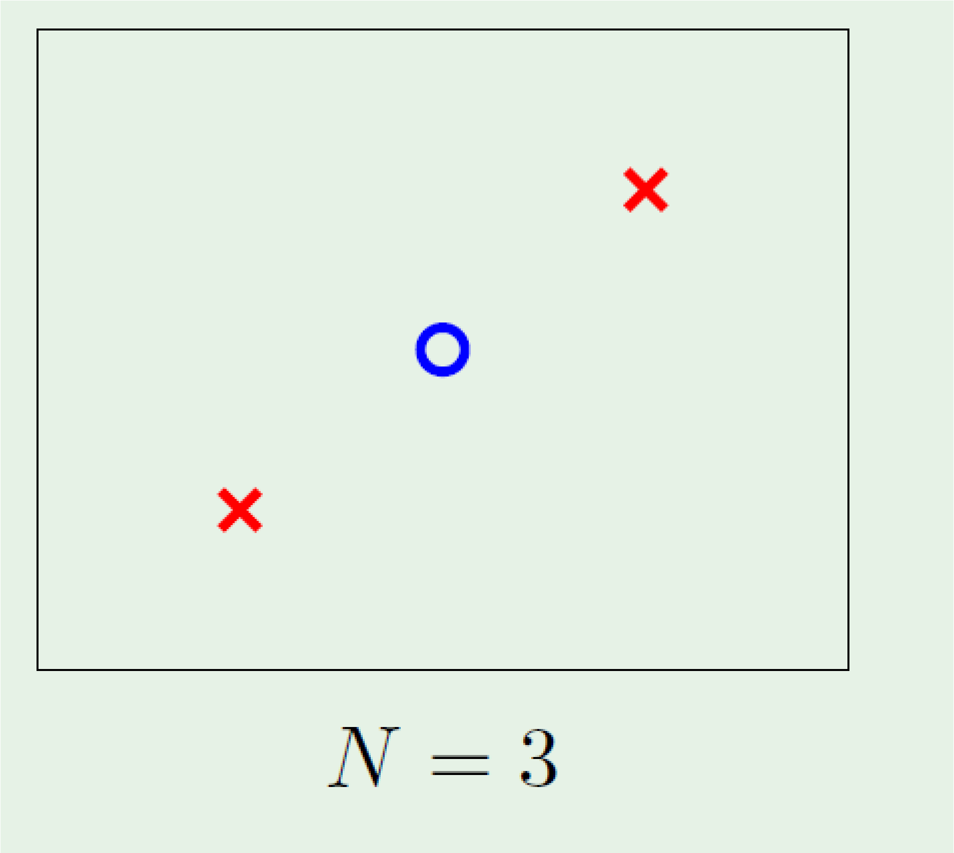
N=3

$m_{H(3)} = 8$



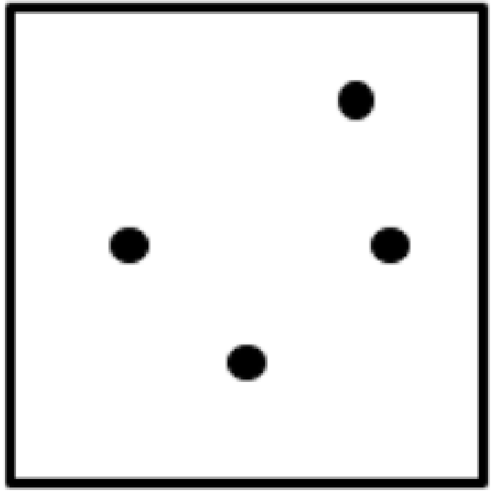
Growth function-Perceptron

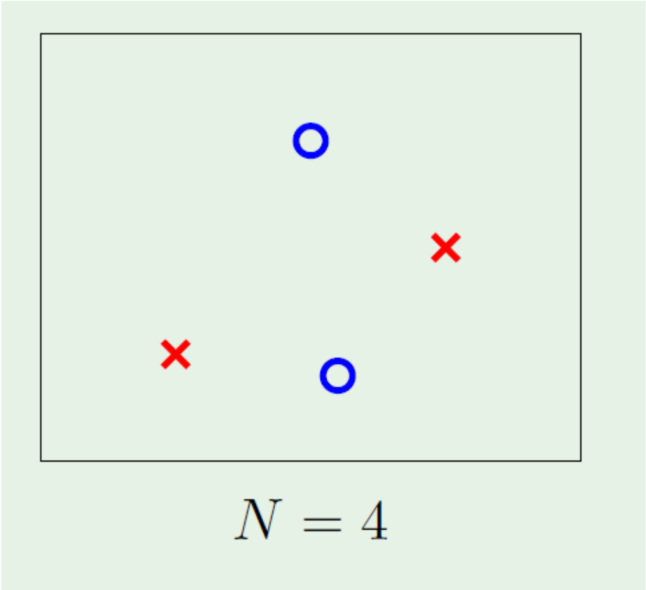
N=3 (co-linear points)



Growth function-Perceptron

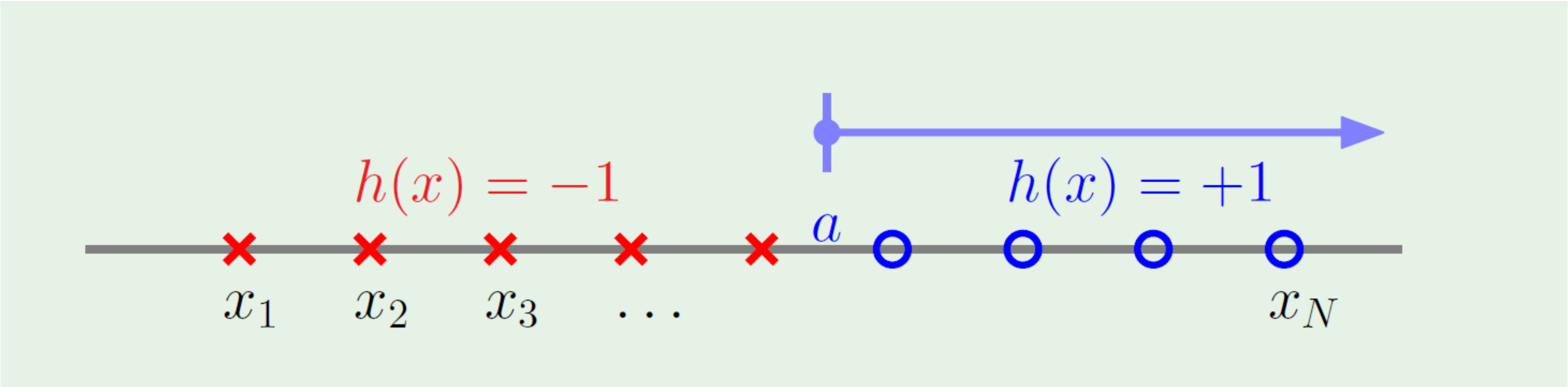
$m_{H(4)} = 14$





Growth function- Positive rays

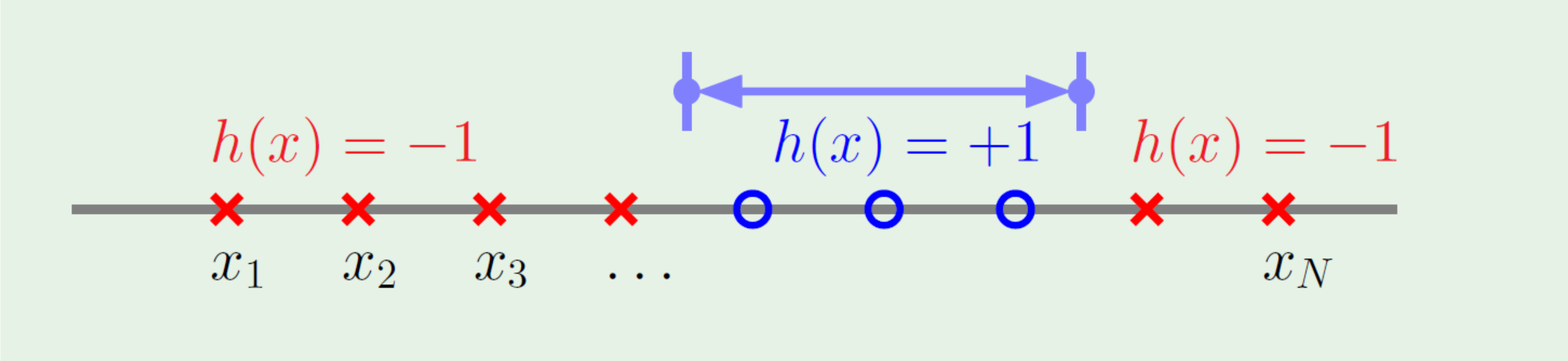
- H consists of all hypotheses h of the form: h(x)=sign(x-a)



- $m_{H(_N)} = \text{N} + 1$

Growth function- Positive intervals

- H consists of all hypotheses in one dimension that returns +1 within some interval and -1 otherwise.
- Each hypothesis is specified by the two end values of the interval (a,b).



- $m_{H}(N) = \binom{N+1}{2} + 1 = \frac{1}{2}N^2 + \frac{1}{2}N + 1$

Convex sets

A set is convex if the line between any two points in the set entirely lies within the set.

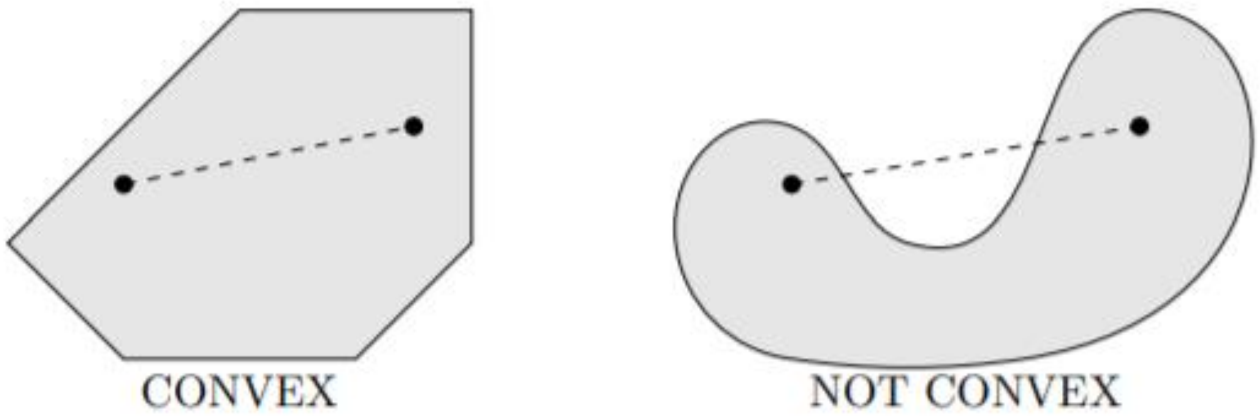
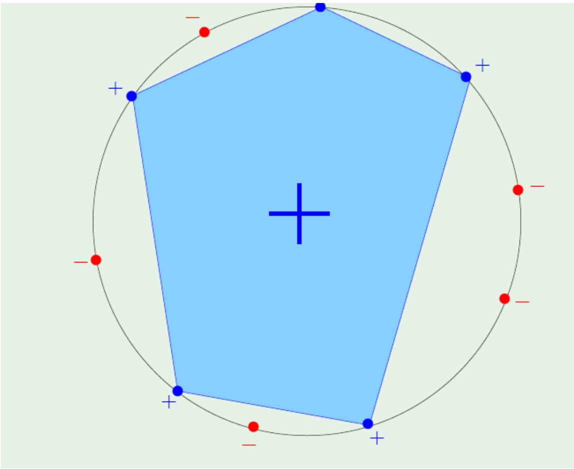


Image source: https://faculty.math.illinois.edu/~mlavrov/docs/484-spring-2019/ch2lec1.pdf

Growth function- Convex sets

- H consists of all the hypotheses in two dimensions that are positive inside a convex set and negative elsewhere.
- Choose N points on the circumference of a circle.
- Connect positive points with a polygon.



- $m_{H(N)} = 2^N$
- H shatters these N points.

Breakpoint

- If no data set of size k can be shattered by H, then k is said to be a breakpoint for H.
- If k is a breakpoint then:

$$m_{H(k)} < 2^k$$

Breakpoint Examples

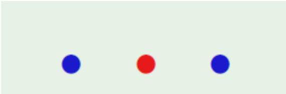
- For 2D perceptron:

  k=4

- For the 1D positive rays:

k=2 

- For the 1D positive interval:

k=3 

- For the convex sets:

  k=∞

The VC Dimension

- The VC dimension of a hypothesis set H denoted by $d_{vc}(H)$ is the largest value of N for which $m_{H(N)} = 2^N$.

- $d_{vc(H)} = k - 1$

- If there is no break point for the hypothesis set H, $m_{H(N)} = 2^N \ \forall N$, then $d_{vc}(H)$=∞.

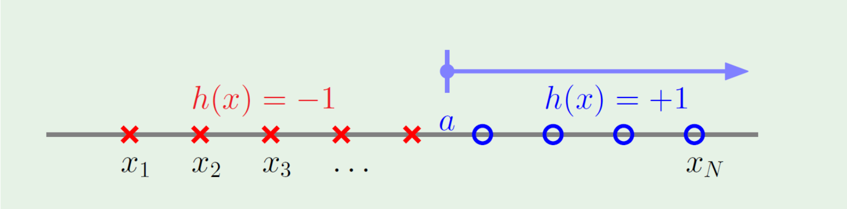
VC dimension-examples

- The VC dimension for 2D perceptron is $d_{vc(H)}$ =3.

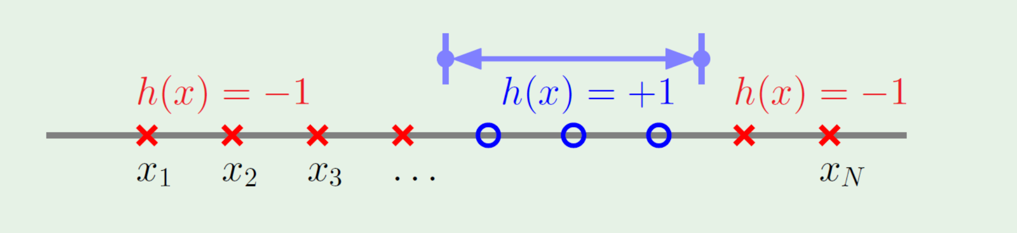
- The VC dimension for d-dimension perceptron is $d_{vc(H)}$ =d+1.

VC dimension-examples (cont.)

- The VC dimension for positive rays $d_{vc(H)}$ =1.



- The VC dimension for positive intervals $d_{vc(H)} = 2$.



- VC dimension can be interpreted as the effective number of parameters (degrees of freedom).

Theorem

- If H has a break point, then $m_{H(N)}$ is bounded by a polynomial in N.

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

$$\boxed{m_{H(N)} \leq \sum_{i=0}^{d_{vc}(H)} \binom{N}{i}}$$

VC-Generalization bound for Infinite hypothesis set

The VC inequality using the growth function instead of M:

$$\Pr[|Ein(g) - Eout(g)| > \varepsilon] \leq 4m_{H(2N)}e^{-\frac{1}{8}\varepsilon^2 N}$$

VC Generalization bound

- The VC inequality:

$$\Pr[|Ein(g) - Eout(g)| > \varepsilon] \leq 4m_{H(2N)}e^{-\frac{1}{8}\varepsilon^2 N}$$

- Thus, with probability at least 1-δ where $\delta = 4m_{H(2N)}e^{-\frac{1}{8}\varepsilon^2 N}$:

$$Eout(g) \leq Ein(g) + \varepsilon$$

- Accordingly, the VC generalization bound:

$$\boxed{Eout(g) \leq Ein(g) + \sqrt{\frac{8}{N}\ln(\frac{4m_{H(2N)}}{\delta})}}$$

- If VC dimension is finite, then the growth function $m_{H(2N)}$ is polynomial, and the generalization error converges to zero as N increases.

Sample Complexity

- The sample complexity means the number of training examples N needed to achieve a certain
- generalization performance.

- The generalization performance is characterized by two parameters:

ε: Error tolerance defines the allowed generalization error

δ: Defines how often the error tolerance ε is violated.

Sample Complexity (cont.)

- To get a generalization error $\leq \varepsilon$:

$$\sqrt{\frac{8}{N}\ln(\frac{4m_{H(2N)}}{\delta})} \leq \varepsilon$$

- Then, the sample complexity N to achieve that generalization error would be:

$$\boxed{N \geq \frac{8}{\varepsilon^{2}}\ln\left(\frac{4m_{H(2N)}}{\delta}\right)}$$

which if function of N, solve it using numerical iterative methods.

As a rule of thumb $N \geq 10\, d_{vc(H)}$

Model Complexity

- With probability at least *1-δ:*

$$Eout(g) \leq Ein(g) + \sqrt{\frac{8}{N}\ln(\frac{4m_{H}(2N)}{\delta})}$$

- With fixed N (number of training samples), the term $\sqrt{\frac{8}{N}\ln(\frac{4m_{H}(2N)}{\delta})}$ can be regarded as model complexity:

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

Thus, with probability at least *1-δ:*

$$\boxed{Eout(g) \leq Ein(g) + \Omega(N,H,\delta)}$$

Model complexity vs. generalization error Trade-off

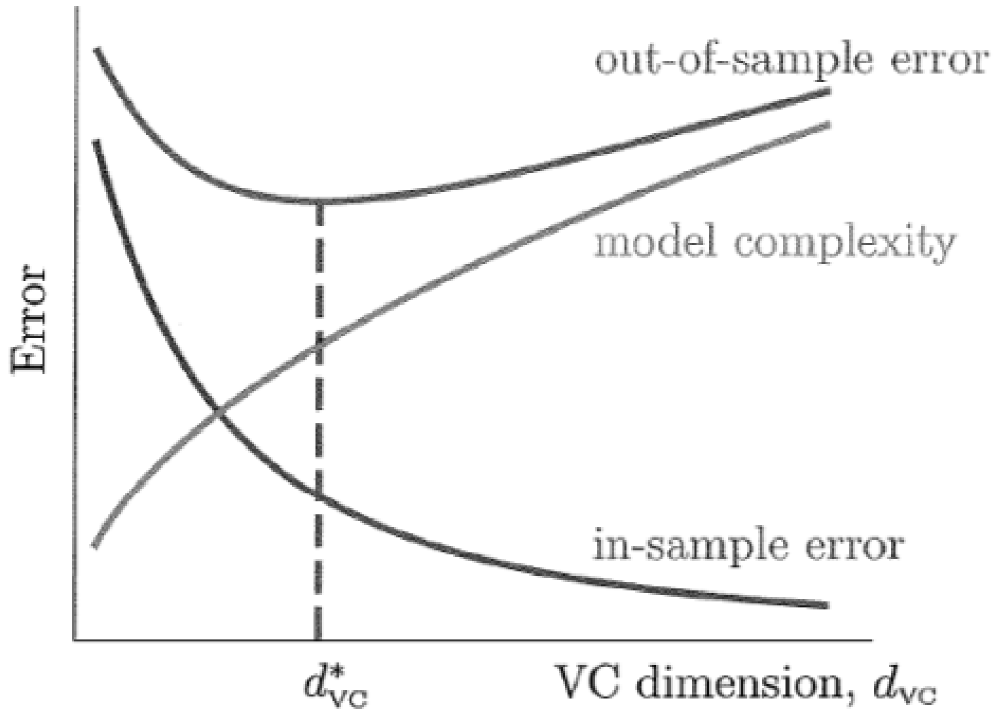
Increases as dvc increases (complex models)

$$Eout(g) \le \underbrace{Ein(g)}_{\text{Decreases as dvc increases (complex models)}} + \sqrt{\frac{8}{N}\ln\left(\frac{4m_{H(2N)}}{\delta}\right)}$$

- The more complex H, the higher $m_{H(2N)}$ and the generalization error would be larger (worse).
- However, the more complex H, the less the in-sample error.

Generalization Error

- A very simple model with low d_{vc}, will not fit the training data well and will have a high in-sample error.
- A more complex learning model with higher d_{vc} would fit the training data better, resulting in a lower in-sample error, but the generalization will be worse.
- Some intermediate d^*_{vc} represents a trade-off between the two errors.



Ein vs. Eout

- Ein is the error on the training data. (in-sample error)
- Eout is the error over the entire input space X. (out of sample error)

- To estimate Eout, we should use new test points that are never used for training.

Estimating Eout in practice

- The VC bound is loose, we need a more accurate estimate of Eout for real-world applications.

Evaluate a sample estimate for Eout as follows:

- Use a fresh new test set of size K not involved in the training process.
- Test the final hypothesis g on the test set and report Etest.

- However, what about the generalization error between Etest and Eout?

We can apply Hoeffding's Inequality as g is not affected by test data.

$$\boxed{P(|Etest(g) - Eout(g)| > \varepsilon) \le 2e^{-2\varepsilon^2 K}}$$

where K is the test set size.

Summary

- Dichotomies
- Growth function
- Breakpoint
- VC dimension
- VC generalization bound for infinite hypotheses
- Sample complexity
- Model Complexity and trade-off between in-sample and generalization error
- Estimate Eout in practice