Learning Theory: Why ML Works

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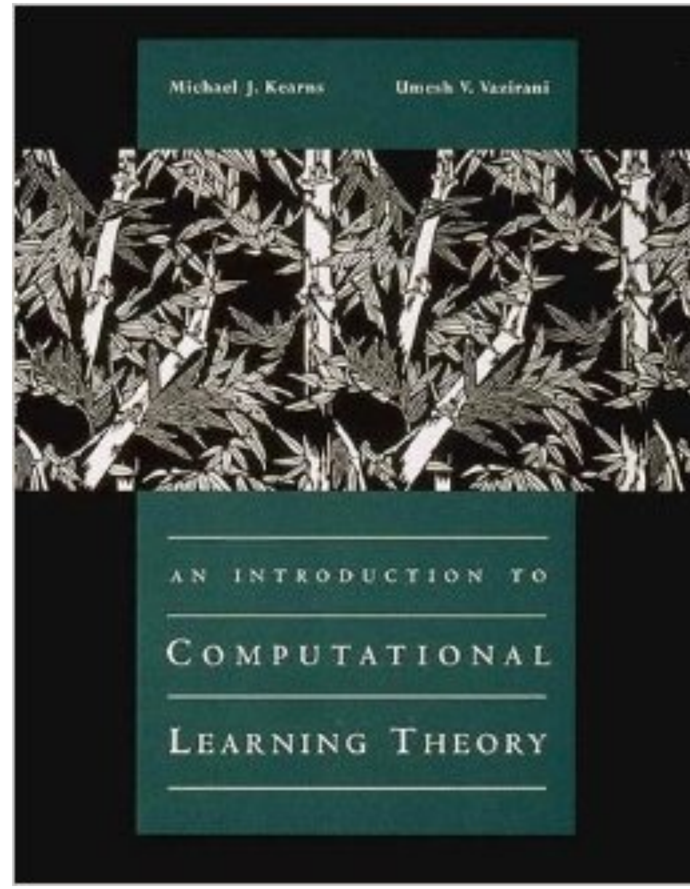
Computational Learning Theory

Entire subfield devoted to the mathematical analysis of machine learning algorithms

Has led to several practical methods:

- PAC (probably approximately correct) learning → boosting
- VC (Vapnik–Chervonenkis) theory → support vector machines



Annual conference: Conference on Learning Theory (COLT)

Computational Learning Theory

Fundamental Question: What general laws constrain inductive learning?

Seeks theory to relate:

- Probability of successful learning
- Number of training examples
- Complexity of hypothesis space
- Accuracy to which target function is approximated
- Manner in which training examples should be presented

Sample Complexity

Assume that $f : \mathcal{X} \mapsto \{0, 1\}$ is the target concept

How many training examples are sufficient to learn the target concept f ?

1. If learner proposed instances as queries to teacher
   - Learner proposes instance x, teacher provides $\mathrm{f}(\mathrm{x})$
2. If teacher (who knows f) provides training examples
   - Teacher provides labeled examples in form $<\mathrm{x}, \mathrm{f}(\mathrm{x})>$
3. If some random process (e.g., nature) proposes instances
   - Instance x generated randomly, teacher provides $\mathrm{f}(\mathrm{x})$

Based on slide by Tom Mitchell

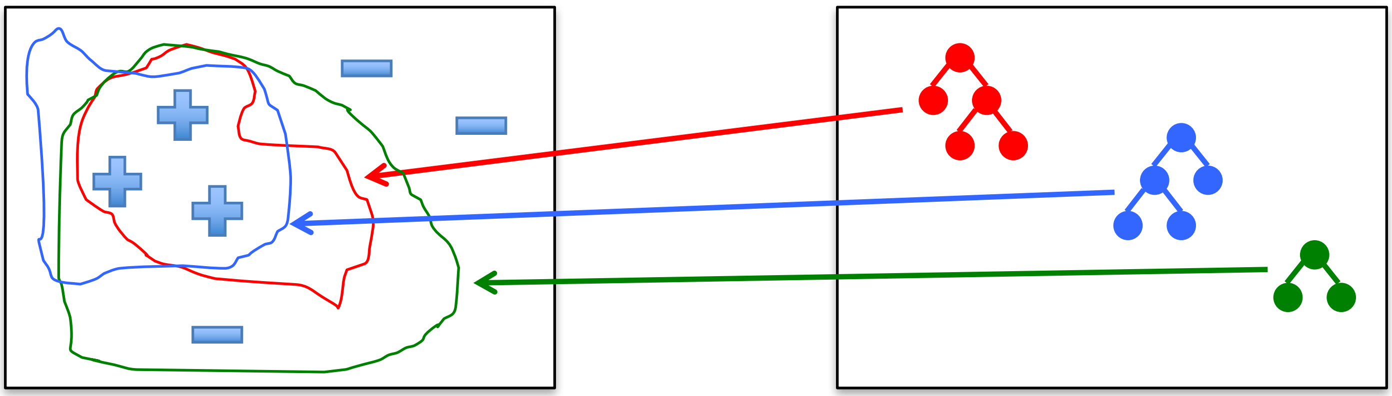
Function Approximation: The Big Picture

Instance Space $\mathcal{X} = \{0,1\}^d$

$\boldsymbol{x} = \langle x_1, x_2, \ldots, x_d \rangle \in \mathcal{X}$

Hypothesis Space

$H = \{h \mid h : \mathcal{X} \mapsto \{0,1\}\}$



if $d = 20$, $|\mathcal{X}| = 2^{20}$

$|h| = 2^{|\mathcal{X}|} = 2^{2^{20}}$

- How many labeled instances are needed to determine which of the $2^{2^{20}}$ hypotheses are correct?
  - <u>All</u> 2^{20} instances in $\mathcal{X}$ must be labeled!
- Generalizing beyond the training data (inductive inference) is impossible unless we add more assumptions (e.g., priors over H)

Based on example by Tom Mitchell

Bias-Variance Decomposition of Squared Error

- Assume that $y = f(\boldsymbol{x}) + \epsilon$
  - Noise ϵ is sampled from a normal distribution with 0 mean and variance σ^2: $\epsilon \sim N(0, \sigma^2)$
  - Noise lower-bounds the performance (error) we can achieve

- Recall the following objective function:

$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \left(y^{(i)} - h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) \right)^2$$

- We can view this as an approximation of the expected value of the squared error: $\mathrm{E} \left(y - h_{\boldsymbol{\theta}} \left(\boldsymbol{x} \right) \right)^2$

Bias-Variance Decomposition of Squared Error

$$
\begin{aligned}
\mathrm{E}[(y - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] &= \mathrm{E}[(y - f(\boldsymbol{x}) + f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&= \mathrm{E}[(y - f(\boldsymbol{x}))^2] + \mathrm{E}[(f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&\qquad + 2\,\mathrm{E}[(f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))(y - f(\boldsymbol{x}))] \\
&= \mathrm{E}[(y - f(\boldsymbol{x}))^2] + \mathrm{E}[(f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&\qquad + 2\left(\cancel{\mathrm{E}[f(\boldsymbol{x}) h_{\boldsymbol{\theta}}(\boldsymbol{x})]} + \cancel{\mathrm{E}[y f(\boldsymbol{x})]} - \cancel{\mathrm{E}[y h_{\boldsymbol{\theta}}(\boldsymbol{x})]} - \cancel{\mathrm{E}[f(\boldsymbol{x})^2]}\right)
\end{aligned}
$$

cancels cancels

Therefore,

$$
\begin{aligned}
\mathrm{E}[(y - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] &= \mathrm{E}[(y - f(\boldsymbol{x}))^2] + \mathrm{E}[(f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&= \mathrm{E}[\epsilon^2] + \mathrm{E}[(f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2]
\end{aligned}
$$

This is actually $\mathrm{var}(\epsilon)$, since mean is 0

Aside:
Definition of Variance
$\mathrm{var}(z) = \mathrm{E}[(z - \mathrm{E}[z])^2]$

Bias-Variance Decomposition of Squared Error

$$
\begin{aligned}
\mathrm{E}[(y - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] &= \mathrm{var}(\epsilon) + \mathrm{E}[(f(\boldsymbol{x}) - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&= \mathrm{var}(\epsilon) + \mathrm{E}[(f(\boldsymbol{x}) - \mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})] + \mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})] - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&= \mathrm{var}(\epsilon) + \mathrm{E}[(f(\boldsymbol{x}) - \mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})])^2] + \mathrm{E}[(\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})] - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&\qquad + 2\mathrm{E}[(\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})] - h_{\boldsymbol{\theta}}(\boldsymbol{x}))(f(\boldsymbol{x}) - \mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})])] \\
&= \mathrm{var}(\epsilon) + \mathrm{E}[(f(\boldsymbol{x}) - \mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})])^2] + \mathrm{E}[(\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})] - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] \\
&\qquad + 2\left(\cancel{\mathrm{E}[f(\boldsymbol{x})\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})]]} - \cancel{\mathrm{E}[\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})]^2]} - \cancel{\mathrm{E}[f(\boldsymbol{x})h_{\boldsymbol{\theta}}(\boldsymbol{x})]} + \cancel{\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})]]}\right)
\end{aligned}
$$

cancels cancels

Therefore,

$$
\mathrm{E}[(y - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] = \underbrace{\mathrm{var}(\epsilon)}_{\text{noise}} + \underbrace{\mathrm{E}[(f(\boldsymbol{x}) - \mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})])^2]}_{\text{bias}} + \underbrace{\mathrm{E}[(\mathrm{E}[h_{\boldsymbol{\theta}}(\boldsymbol{x})] - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2]}_{\text{variance}}
$$

$$
\mathrm{E}[(y - h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2] = \mathrm{bias}(h_{\boldsymbol{\theta}}(\boldsymbol{x}))^2 + \mathrm{var}(h_{\boldsymbol{\theta}}(\boldsymbol{x})) + \sigma^2
$$

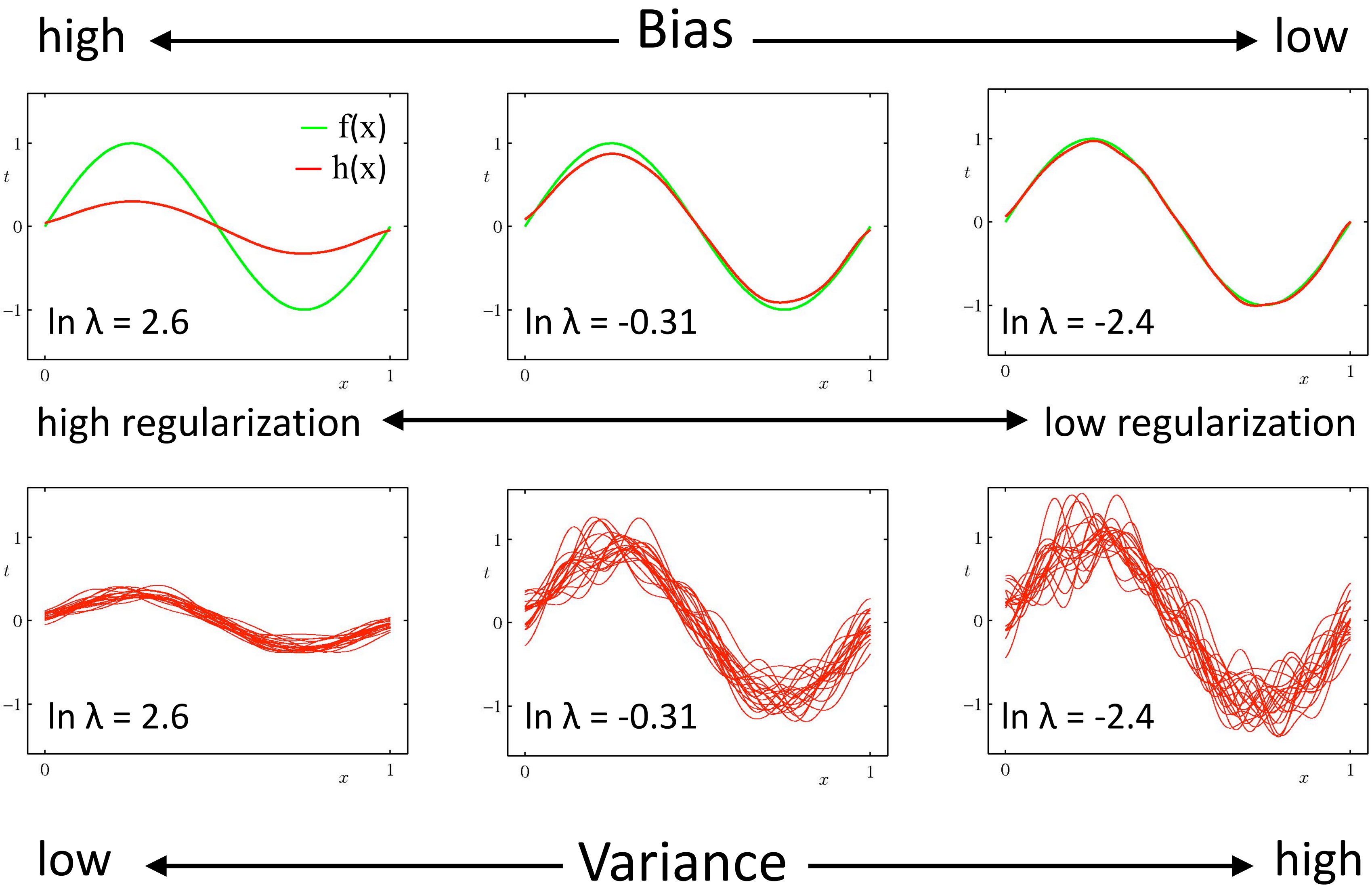
Regularization

- Linear regression objective function

$$J(\boldsymbol{\theta}) = \underbrace{\frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2}_{\text{model fit to data}} + \underbrace{\frac{\lambda}{2}\sum_{j=1}^{d}\theta_j^2}_{\text{regularization}}$$

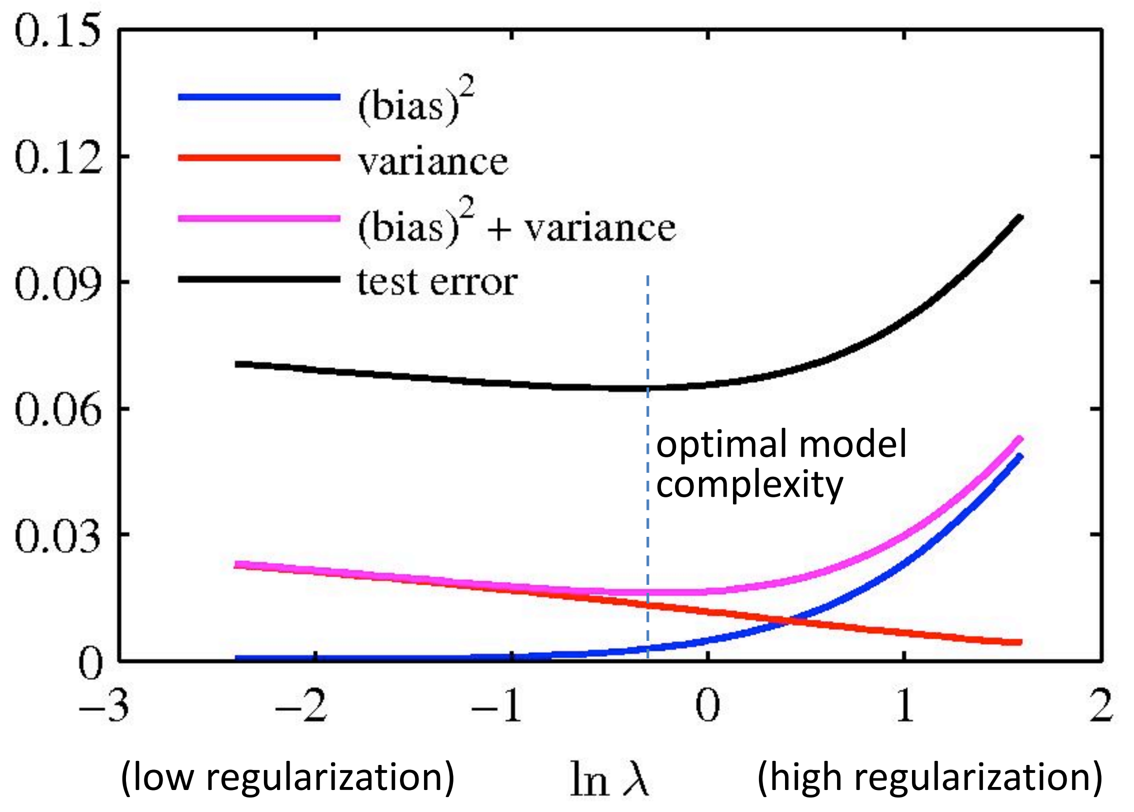
  – λ is the regularization parameter ($\lambda \geq 0$)

Illustration of Bias-Variance



Figures provided by by Max Welling

Illustration of Bias-Variance



- Training error drives down bias, but ignores variance

Figure provided by by Max Welling

A Way to Choose the Best Model

- It would be really helpful if we could get a guarantee of the following form:

$$\text{testingError} \leq \text{trainingError} + f(n, h, p)$$

  n = size of training set

  h = measure of the model complexity

  p = the probability that this bound fails

  We need p to allow for really unlucky test sets

- Then, we could choose the model complexity that minimizes the bound on the test error

A Weird Measure of Model Complexity

- Suppose that we pick n data points and assign labels of + or – to them at random
- If our model class (e.g., a decision tree, polynomial regression of a particular degree, etc.) can learn any association of labels with data, it is too powerful!

More power: can model more complex functions, but may overfit

Less power: won't overfit, but limited in what it can represent

- **Idea**: characterize the power of a model class by asking how many data points it can learn perfectly for all possible assignments of labels
  – This number of data points is called the Vapnik-Chervonenkis (VC) dimension

VC Dimension

- A measure of the power of a particular class of models
  - It does not depend on the choice of training set

- The VC dimension of a model class is the maximum number of points that can be arranged so that the class of models can shatter those points

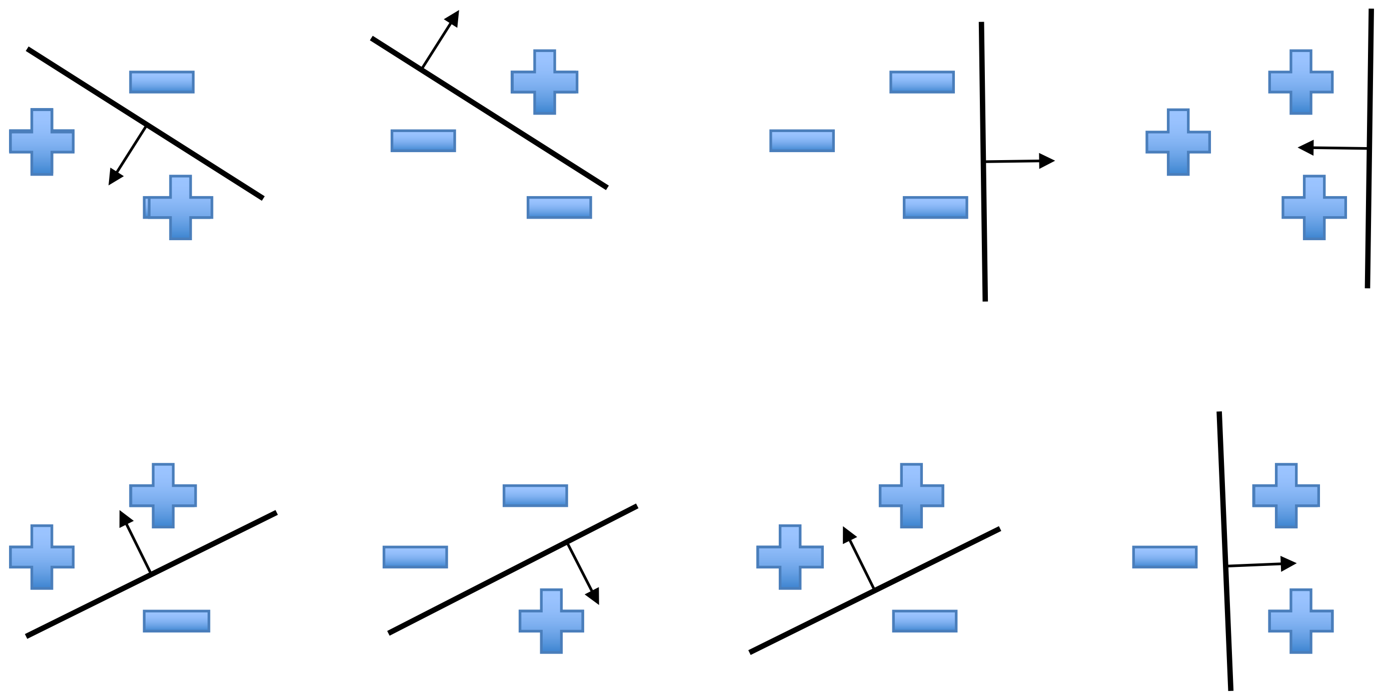
Definition: a model class can shatter a set of points

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(r)}$$

if for <u>every</u> possible labeling over those points, there exists a model in that class that obtains zero training error

An Example of VC Dimension

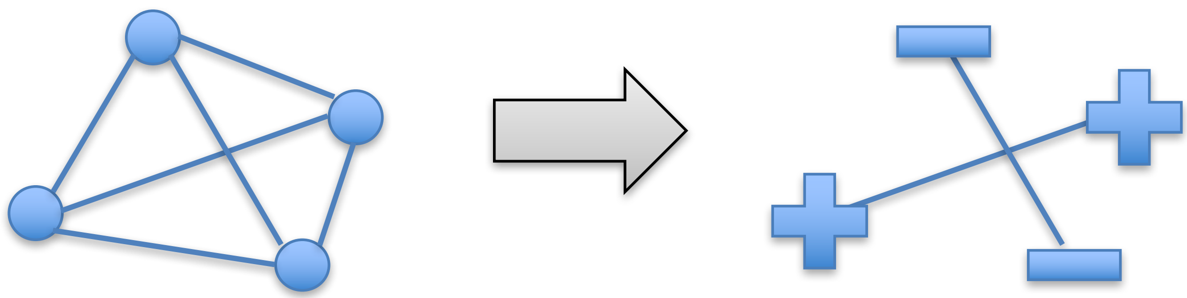
- Suppose our model class is a hyperplane
- Consider all labelings over three points in $\mathbb{R}^2$



- In $\mathbb{R}^2$, we can find a plane (i.e., a line) to capture any labeling of 3 points. A 2D hyperplane shatters 3 points

An Example of VC Dimension

- But, a 2D hyperplane cannot deal with some labelings of four points:



Connect all pairs of points; two lines will always cross

Can’t separate points if the pairs that cross are the same class

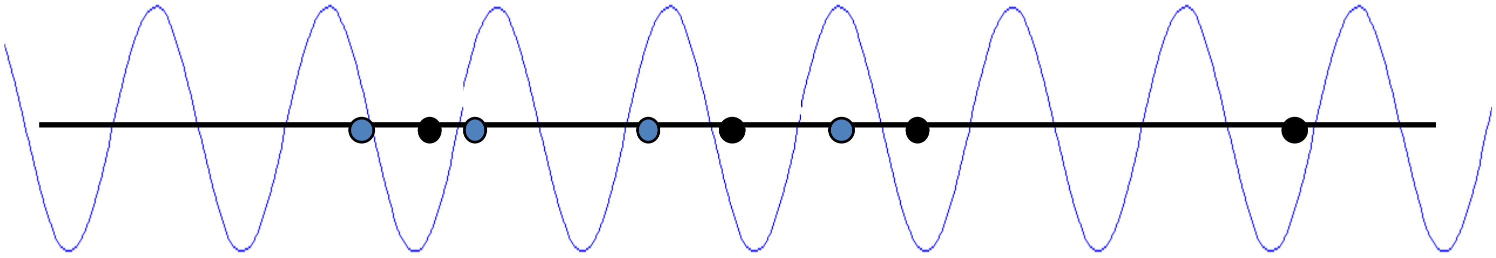
- Therefore, a 2D hyperplane cannot shatter 4 points

Some Examples of VC Dimension

- The VC dimension of a hyperplane in 2D is 3.
  - In d dimensions it is $d+1$
    - It's just a coincidence that the VC dimension of a hyperplane is almost identical to the # parameters needed to define a hyperplane

- A sine wave has infinite VC dimension and only 2 parameters!
  - By choosing the phase & period carefully we can shatter any random set of 1D data points (except for nasty special cases)

$$h(x) = a\sin(bx)$$



Assumptions

- Given some model class (which defines the hypothesis space H)
- Assume all training points were drawn i.i.d from distribution $\mathcal{D}$
- Assume all future test points will be drawn from $\mathcal{D}$

Definitions:

$$R(\boldsymbol{\theta}) = \text{testError}(\boldsymbol{\theta}) = \underbrace{E\left[\frac{1}{2}|y - h_{\boldsymbol{\theta}}(\boldsymbol{x})|\right]}_{\text{probability of misclassification}}$$

"official" notation

notation we'll use

$$R^{\text{emp}}(\boldsymbol{\theta}) = \text{trainError}(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{2}\left|y^{(i)} - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right|$$

A Probabilistic Guarantee of Generalization Performance

Vapnik showed that with probability (1 –η):

$$\mathrm{testError}(\boldsymbol{\theta}) \leq \mathrm{trainError}(\boldsymbol{\theta}) + \sqrt{\frac{h(\log(2n/h)+1) - \log(\eta/4)}{n}}$$

n = size of training set

h = VC dimension of model class

η= the probability that this bound fails

- So, we should pick the model with the complexity that minimizes this bound
  - Actually, this is only sensible if we think the bound is fairly tight, which it usually isn’t
  - The theory provides insight, but in practice we still need some witchcraft

Take Away Lesson

Suppose we find a model with a low training error...

- If hypothesis space H is very big (relative to the size of the training data n), then we most likely overfit

- If the following holds:
  - H is sufficiently constrained in size
  - and/or the size of the training data set n is large,

  then low training error is likely to be evidence of low generalization error