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 $f(x)$

2. If teacher (who knows $f$) provides training examples
   - Teacher provides labeled examples in form $<x, f(x)>$

3. If some random process (e.g., nature) proposes instances
   - Instance $x$ generated randomly, teacher provides $f(x)$

Based on slide by Tom Mitchell
Function Approximation: The Big Picture

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

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

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?
  – All $2^{20}$ 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 $y = f(x) + \epsilon$
  
  – Noise $\epsilon$ is sampled from a normal distribution with 0 mean and variance $\sigma^2$: $\epsilon \sim N(0, \sigma^2)$
  
  – Noise lower-bounds the performance (error) we can achieve

• Recall the following objective function:

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

• We can view this as an approximation of the expected value of the squared error: $E \left( y - h_\theta (x) \right)^2$
Bias-Variance Decomposition of Squared Error

\[
E[(y - h_\theta(x))^2] = E[(y - f(x) + f(x) - h_\theta(x))^2]
\]
\[
= E[(y - f(x))^2] + E[(f(x) - h_\theta(x))^2]
\]
\[
+ 2 E[(f(x) - h_\theta(x))(y - f(x))]
\]
\[
= E[(y - f(x))^2] + E[(f(x) - h_\theta(x))^2]
\]
\[
+ 2\left[E[f(x)h_\theta(x)] + E[yf(x)] - E[yh_\theta(x)] - E[f(x)^2]\right]
\]

Therefore,

\[
E[(y - h_\theta(x))^2] = E[(y - f(x))^2] + E[(f(x) - h_\theta(x))^2]
\]
\[
= E[\epsilon^2] + E[(f(x) - h_\theta(x))^2]
\]

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

This is actually \( \text{var}(\epsilon) \), since mean is 0
Bias-Variance Decomposition of Squared Error

\[
E[(y - h_\theta(x))^2] = var(\epsilon) + E[(f(x) - h_\theta(x))^2]
\]
\[
= var(\epsilon) + E[(f(x) - E[h_\theta(x)] + E[h_\theta(x)] - h_\theta(x))^2]
\]
\[
= var(\epsilon) + E[(f(x) - E[h_\theta(x)])^2] + E[(E[h_\theta(x)] - h_\theta(x))^2]
\]
\[
\quad + 2E[(E[h_\theta(x)] - h_\theta(x))(f(x) - E[h_\theta(x)])]
\]
\[
= var(\epsilon) + E[(f(x) - E[h_\theta(x)])^2] + E[(E[h_\theta(x)] - h_\theta(x))^2]
\]
\[
\quad + 2(E[f(x)E[h_\theta(x)]] - E[E[h_\theta(x)]^2] - E[f(x)h_\theta(x)] + E[h_\theta(x)E[h_\theta(x)]])
\]

Therefore,

\[
E[(y - h_\theta(x))^2] = var(\epsilon) + E[(f(x) - E[h_\theta(x)])^2] + E[(E[h_\theta(x)] - h_\theta(x))^2]
\]

\[
E[(y - h_\theta(x))^2] = bias(h_\theta(x))^2 + var(h_\theta(x)) + \sigma^2
\]
Regularization

- Linear regression objective function

\[
J(\theta) = \frac{1}{2n} \sum_{i=1}^{n} \left( h_\theta(x^{(i)}) - y^{(i)} \right)^2 + \frac{\lambda}{2} \sum_{j=1}^{d} \theta_j^2
\]

- model fit to data
- regularization

- \( \lambda \) 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
A Way to Choose the Best Model

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

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

\(n = \text{size of training set}\)
\(h = \text{measure of the model complexity}\)
\(p = \text{the probability that this bound fails}\)

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 $x^{(1)}, x^{(2)}, \ldots, x^{(r)}$ if for every possible labeling over those points, there exists a model in that class that obtains zero training error

Based on Andrew Moore’s tutorial slides
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

Based on slides by Geoff Hinton
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 $D$
• Assume all future test points will be drawn from $D$

Definitions:

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

“official” notation

probability of misclassification

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

notation we’ll use

Based on Andrew Moore’s tutorial slides
A Probabilistic Guarantee of Generalization Performance

Vapnik showed that with probability $(1 - \eta)$:

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

- $n = \text{size of training set}$
- $h = \text{VC dimension of model class}$
- $\eta = \text{the probability that this bound fails}$

- 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.