Learning Theory

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Content

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- The Association for Computational Learning (ACL) is in charge of the organization of the Conference on Learning Theory (COLT).

Figure: http://www.learningtheory.org

Learning Theory

- The emphasis is on rigorous mathematical analysis using tools from:

Information Theory
Probability
Optimization
Statistics
Geometry

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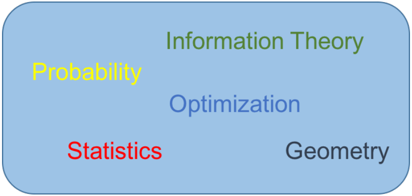

- While theoretically rooted, learning theory puts a strong emphasis on efficient computation as well.

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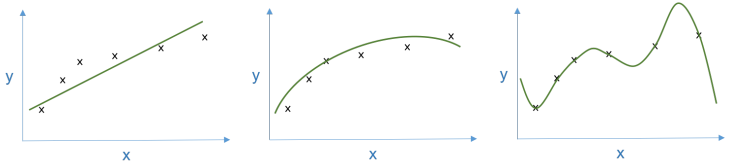
- Important results in this field are usually published in:
  - Conference on Learning Theory (COLT).
  - Journal of Machine Learning Research (JMLR).

Bias Vs Variance

- When talking about linear regression, we wonder whether to fit a simple model such as the linear $y = \theta_0 + \theta_1 x$, or a more complex model such as the polynomial $y = \theta_0 + \theta_1 x + \ldots + \theta_5 x^5$.



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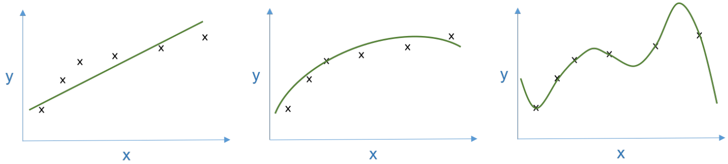

- Given this data set, the 5th order polynomial (rightmost curve) does not result in a good model, because it will not generalize well with other examples.

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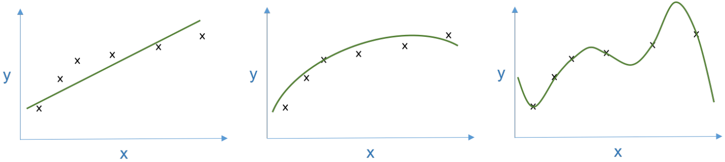

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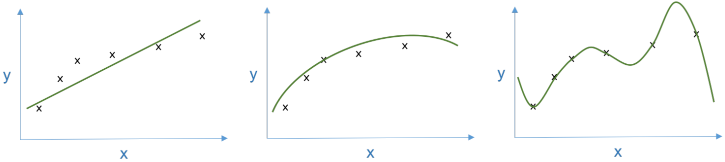

- However, the problems that the two models suffer from are very different.

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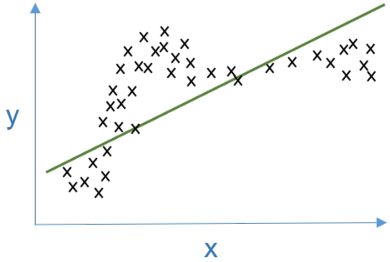
- A linear model might be too simple to capture the structure in the data.



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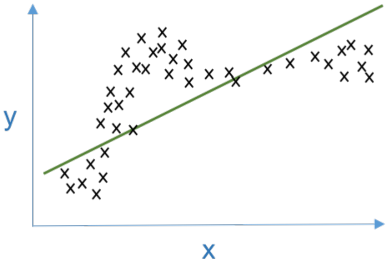
- Thus, for the problem above, the linear model suffers from **large bias**, and may underfit the data: it may fail to capture the structure exhibited by the data.



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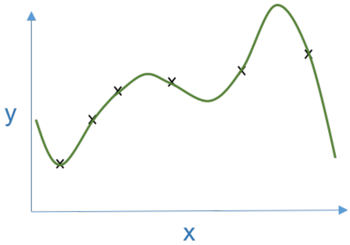
- The **variance** of a model fitting procedure is a second component of the generalization error.
- When fitting a 5th order polynomial, there is a large risk that we're fitting patterns in the data that happened to be present in our small, training set, but that do not reflect the wider pattern of the relationship between x and y.



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- By fitting this spurious pattern in the training set, we might again obtain a model with large generalization error.

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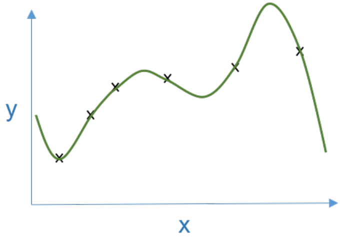

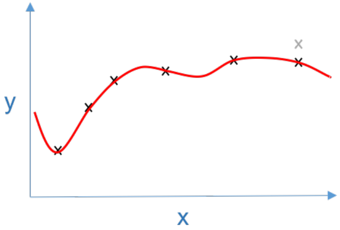

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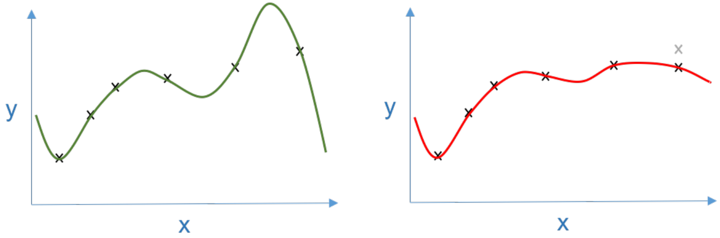

- In this case we say the model has a **large variance**.

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- Therefore, in general we can say that

Model	Parameters	Bias	Variance
Simple	Few	Large	Small
Complex	Many	Small	Large

Bias Vs Variance

- In our example, fitting a quadratic function does better than either of the extremes of a first or a fifth order polynomial.

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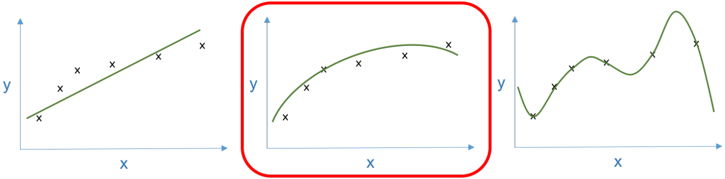

Three learning theory questions

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2. Can we relate the error on the training set to the generalization error?
3. Are there conditions under which we can actually prove that learning algorithms will work well?

Union Bound Lemma

- Let $A_1, A_2, \ldots, A_k$ be k different events (that may not be independent). Then

  $P(A_1 \cup A_2, \cup \ldots \cup A_k) \leq P(A_1) + \ldots + P(A_k)$.

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- In probability theory, the union bound is usually stated as an axiom, but it also makes intuitive sense: The probability of any one of k events happening is at most the sum of the probabilities of the k different events.

Hoeffding Inequality Lemma

- Let $Z_1, \ldots, Z_m$ be m independent and identically distributed (iid) random variables drawn from a Bernoulli(ϕ) distribution. I.e., $P(Z_i = 1) = \phi$, and $P(Z_i = 0) = 1 - \phi$. Let $\hat{\phi} = (1/m)\sum_{i=1}^{m} Z_i$ be the mean of these random variables, and let any $\gamma > 0$ be fixed. Then

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- This lemma, also called the Chernoff bound, say that if we take $\hat{\phi}$ to be our estimate of ϕ, then the probability of our estimate to be far from the true value is small, as long as m is large.

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- We will restrict our attention to the binary classification problem in which the labels are $y \in \{0, 1\}$. However, everything we will say here generalizes to other, including regression and multi-class classification problems.
- We assume we are given a training set $S = \{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$, where the training examples are drawn iid from a probability distribution $\mathcal{D}$.

Empirical Risk Minimization

- For a hypothesis h, we define the **training error** (also called **empirical risk** or **empirical error** in learning theory) to be

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- This is just the fraction of training examples that h missclasifies.

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- Note that we have assumed that the training data was drawn from the same distribution $\mathcal{D}$ with which we are going to evaluate our hypothesis h. This is sometimes also referred to as one of the **PAC** assumptions.

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Of these, the assumption of training and testing on the same distribution, and the assumption of the independently drawn training examples, were the most important.

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- We think of ERM as the most basic learning algorithm. Algorithms such as logistic regression can also be viewed as approximations to ERM.

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- If we were studying neural networks, then we could let $\mathcal{H}$ be the set of all classifiers representable by some neural network architecture.

Hypothesis Class $\mathcal{H}$

- Empirical risk minimization can now be thought of as a minimization over the class of functions $\mathcal{H}$, in which the learning algorithm picks the hypothesis:

  $\hat{h} = \arg\min_{h \in \mathcal{H}} \hat{\varepsilon}(h)$.

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- To give some guarantees on the generalization error of $\hat{h}$, we will:
  1. Show that $\hat{\varepsilon}(h)$ is a reliable estimate of $\varepsilon(h)$ for all h.
  2. Show that this implies an upper-bound on the generalization error of $\hat{h}$.

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- Since, our training set was drawn iid from $\mathcal{D}$, then Z and the Z_j's have the same distribution.

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- We can apply the Hoeffding inequality and obtain

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- Let A_i denote the event that $|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma$.
- We have seen that for any particular A_i it holds true that $P(A_i) \leq 2\exp(-2\gamma^2 m)$.

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Thus, using the union bound, we have that

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If we substract both sides from 1, we find that

$$P(\neg\exists h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma) = P(\forall h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma)$$

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P(\exists h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma) &= P(A_1 \cup \ldots \cup A_k) \\
&\leq \sum_{i=1}^{k} P(A_i) \\
&\leq \sum_{i=1}^{k} 2\exp(-2\gamma^2 m) \\
&= 2k\exp(-2\gamma^2 m)
\end{aligned}
$$

If we substract both sides from 1, we find that

$$
\begin{aligned}
P(\neg\exists h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma) &= P(\forall h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma) \\
& 1 - 2k\exp(-2\gamma^2 m)
\end{aligned}
$$

The Finite Class $\mathcal{H}$

Thus, the expression

$$P(\forall h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma) \geq 1 - 2k\ \exp(-2\gamma^2 m)$$

The Finite Class $\mathcal{H}$

Thus, the expression

$$P(\forall h \in \mathcal{H},\ |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma) \geq 1 - 2k\,\exp(-2\gamma^2 m)$$

means that, with probability at least $1 - 2k\,\exp(-2\gamma^2 m)$, we have that $\varepsilon(h)$ will be within γ of $\hat{\varepsilon}(h)$ for all $h \in \mathcal{H}$.

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means that, with probability at least $1 - 2k\ \exp(-2\gamma^2 m)$, we have that $\varepsilon(h)$ will be within γ of $\hat{\varepsilon}(h)$ for all $h \in \mathcal{H}$.

This is called a **uniform convergence** result, because this is a bound that holds simultaneously for all $h \in \mathcal{H}$.

The Finite Class $\mathcal{H}$

- Given γ and some $\delta > 0$, how large must m be before we can guarantee that with probability at least $1 - \delta$, the training error will be within γ of the generalization error?

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- By setting $\delta = 2k \exp(-2\gamma^2 m)$ and solving for m, we find that

  $m \geq \frac{1}{2\gamma^2} \log \frac{2k}{\delta}$,

  then with probability at least $1 - \delta$, we have that $|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma$ for all $h \in \mathcal{H}$.

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  then with probability at least $1 - \delta$, we have that $|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma$ for all $h \in \mathcal{H}$.
- This bound tells us how many training examples we need in order to make a guarantee. The training set size m that a certain method or algorithm requires in order to achieve a certain level of performance is also called the algorithm's sample complexity.

The Finite Class $\mathcal{H}$

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- Similarly, if we fix m and δ and solve for γ, we get that with probability $1-\delta$, we have that for all $h \in \mathcal{H}$,

  $$|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \sqrt{\frac{1}{2m} \log \frac{2k}{\delta}}.$$

The Finite Class $\mathcal{H}$

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- In the first and third step we used $|\varepsilon(\hat{h}) - \hat{\varepsilon}(\hat{h})| \leq \gamma$ and $\hat{\varepsilon}(h^*) \leq \varepsilon(h^*) + \gamma$, respectively.

The Finite Class $\mathcal{H}$

- **Theorem.** Let $|\mathcal{H}| = k$, and let any m, δ be fixed. Then with probability at least $1 - \delta$, we have that

$$\varepsilon(\hat{h}) \leq \left(\min_{h \in \mathcal{H}} \varepsilon(h) \right) + 2\sqrt{\frac{1}{2m} \log \frac{2k}{\delta}}$$

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- When we switch from $\mathcal{H}$ to $\mathcal{H}'$ where $\mathcal{H}' \supseteq \mathcal{H}$, the first term can only decrease, and therefore our bias can only decrease.
- However, if k increases, then the second term will would also increase, and therefore the variance would increase as well.

The Finite Class $\mathcal{H}$

- **Corollary.** Let $|\mathcal{H}| = k$, and let any δ, γ be fixed. Then for $\varepsilon(\hat{h}) \leq \min_{h \in \mathcal{H}} \varepsilon(h) + 2\gamma$ to hold with probability at least $1 - \delta$, it suffices that

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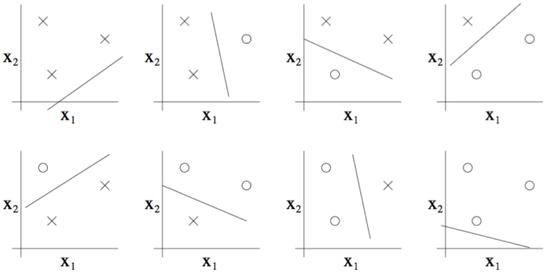
$$\begin{aligned} m &\geq \frac{1}{2\gamma^2} \log \frac{2k}{\delta} \\ &= O\left(\frac{1}{\gamma^2} \log \frac{k}{\delta}\right) \end{aligned}$$

Vapnik-Chervonenkis Dimension

- **Definition.** Given a hypothesis class $\mathcal{H}$, we then define its Vapnik-Chervonenkis dimension, written VC($\mathcal{H}$), to be the size of the largest set of points that is shattered by $\mathcal{H}$.



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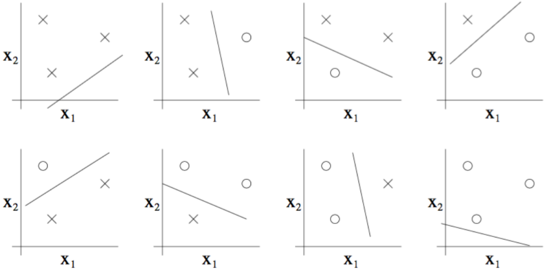

- For a linear classifier in two dimensions, $\mathrm{VC}(\mathcal{H}) = 3$.

The Infinite Class $\mathcal{H}$

- **Theorem.** Let $\mathcal{H}$ be given, and let $d = \mathrm{VC}(\mathcal{H})$. Then with probability at least $1 - \delta$, we have that for all $h \in \mathcal{H}$,

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- In other words, if a hypothesis class has finite VC dimension, then uniform convergence occurs as m becomes large. This allows us to give a bound on $\varepsilon(h)$ in terms of $\varepsilon(h^*)$.

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Thank you!

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