Lecture 1: Theoretical foundations of ML

Pranabendu Misra
Chennai Mathematical Institute

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(based on slides by Madhavan Mukund)

Supervised learning

- Set of possible input instances X

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- Categories C, say $\{0, 1\}$

$x \in X$

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- Build a classification model $M : X \to C$

$M(x) \to \hat{c}(x)$

??

$c(x)$

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- Categories C, say $\{0, 1\}$
- Build a classification model $M : X \to C$
- Restrict the types of models
  - Hypothesis space $\mathcal{H}$ — e.g., linear separators
  - Search for best $M \in \mathcal{H}$

M is a linear fn of x

Very complex fn in DL

Supervised learning

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- Build a classification model $M : X \to C$
- Restrict the types of models
  - Hypothesis space $\mathcal{H}$ — e.g., linear separators
  - Search for best $M \in \mathcal{H}$
- How do we find the best M?
  - Labelled training data (training set)
  - Choose M to minimize error (loss) with respect to the training set
  - Why should M generalize well to arbitrary data?

$\forall x \in S$

$\ell(x) \in C$

$S = \{(x, \ell(x)) \mid x \in X\}$

Suppose we can do this

No free lunch

- ML algorithms minimize training loss (with respect to the training set)

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- Goal is to minimize generalization loss (with respect to all inputs)

$$\text{Train Loss}(M) = \frac{\sum_{x \in S} [1 \text{ if } M(x) \neq f(x)]}{|S|}$$

$$\text{Gen Loss}(M) = \frac{\sum_{x \in \text{all inps}} [\;]}{|\text{all inps}|}$$

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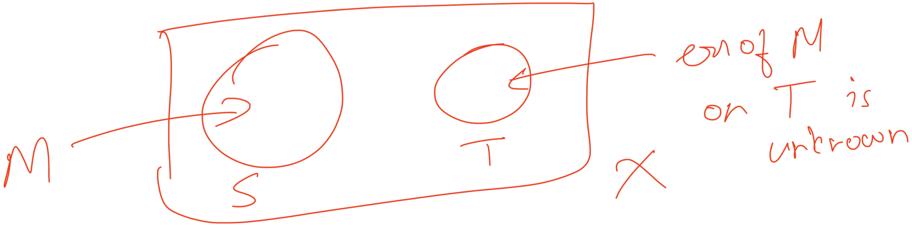
No Free Lunch Theorem [Wolpert, Macready 1997]

Averaged over all possible data distributions, every classification algorithm has the same error rate when classifying previously unobserved points.



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- Is the situation hopeless?
- NFL theorem refers to prediction inputs coming from all possible distributions
- ML assumes training set is representative of overall data
  - Prediction instances follow roughly the same distribution as training set

A theoretical framework for ML

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  - e.g., X is all emails, C is the set of spam emails

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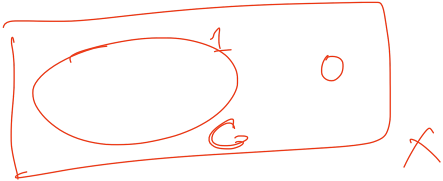
  - e.g., X is all emails, C is the set of spam emails
- X is equipped with a probability distribution D
  - Any random sample from X is drawn using D
  - In particular, training set and test set are constitute of such random samples

Binary Classification



$$\sum_{x \in X} D(x) = 1$$

X → all emails

C → all spam emails

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  - Each $h \in \mathcal{H}$ identifies a subset of X
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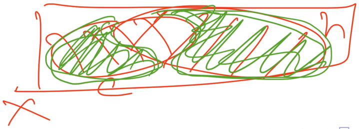
- True error: Probability that h incorrectly classifies $x \in X$ drawn randomly according to D
  - $err_D(h) = \text{Prob}(h \Delta C)$
  - $h \Delta C = (h \setminus C) \cup (C \setminus h)$



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- Training error: Given a (finite) training sample $S \subseteq X$
  - $\text{err}_S(h) = |S \cap (h \Delta C)|/|S|$

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- X, inputs with distribution D
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h ∈ H

Goal

Minimizing training error should correspond to minimizing true error

- Overfitting Low training error but high true error
- Underfitting Cannot achieve low training/true error
- Related to the representational capacity of $\mathcal{H}$
  - How expressive is $\mathcal{H}$? How many different concepts can it capture?
  - Capacity too high — overfitting
  - Capacity too low — underfitting

Probably Approximately Correct (PAC) learning

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  With high probability, the hypothesis h that fits the sample S also fits the concept C approximately correctly

best $h \in H$ wrt S

least train loss

Probably Approximately Correct (PAC) learning

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Theorem (PAC learning guarantee)

Let $\delta, \epsilon > 0$. Let S be a training set of size $n \geq \frac{1}{\epsilon}(\ln|\mathcal{H}| + \ln(1/\delta))$ drawn using D. With probability $\geq 1 - \delta$, every $h \in \mathcal{H}$ with training error zero has true error $< \epsilon$.

- Size of the sample required for PAC guarantee determined by parameters δ, ϵ
  - Smaller δ means higher probability of find a good hypothesis
  - Smaller ϵ means better performance with respect to generalization

Probably Approximately Correct (PAC) learning

Theorem (Uniform convergence)

Let $\delta, \epsilon > 0$. Let S be a training set of size $n \geq \frac{1}{2\epsilon^2}(\ln|\mathcal{H}| + \ln(2/\delta))$ drawn using D. With probability $\geq 1 - \delta$, every $h \in \mathcal{H}$ satisfies $|\mathrm{err}_S(h) - \mathrm{err}_D(h)| \leq \epsilon$.

- Stronger guarantee: even if we cannot achieve zero training error, the additional generalization error is bounded

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VC-Dim($\mathcal{H}$)

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- Other measures of capacity — e.g. VC-dimension of $\mathcal{H}$

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- Other measures of capacity — e.g. VC-dimension
- Analogous convergence theorems in terms of VC-dimension

Overfitting and underfitting

Example: Regression

- $\mathcal{H}_d$ is set of polynomials of degree d

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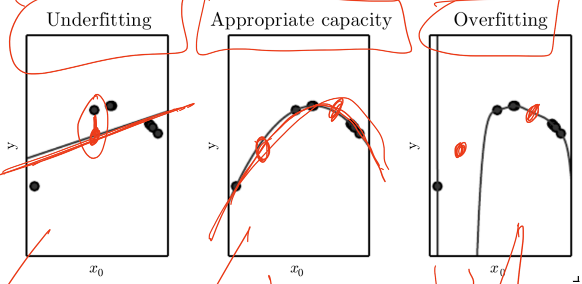

- Random points lying along a quadratic

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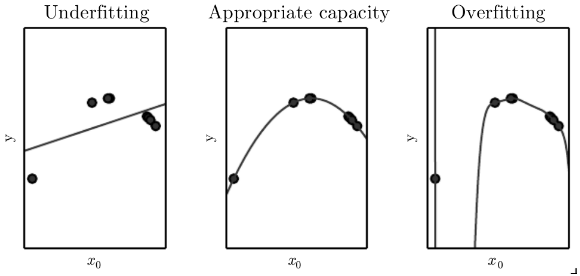

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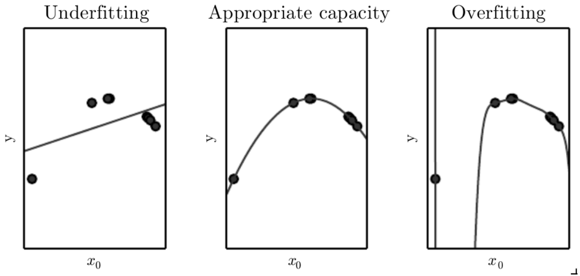

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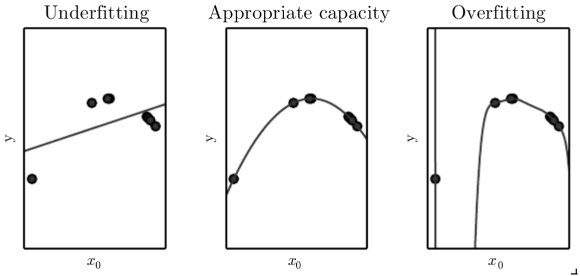

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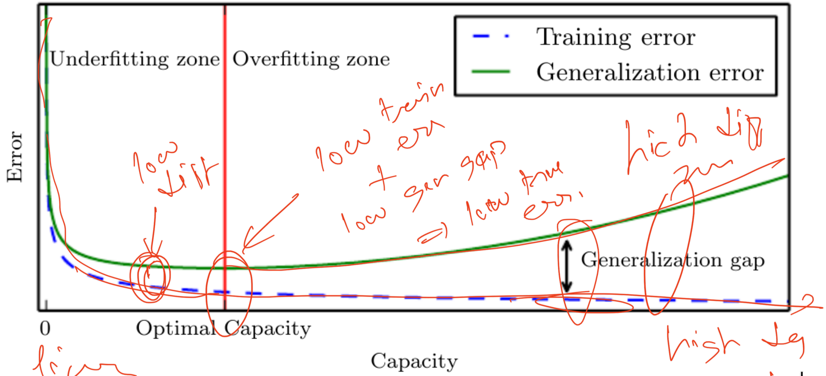
Capacity and error



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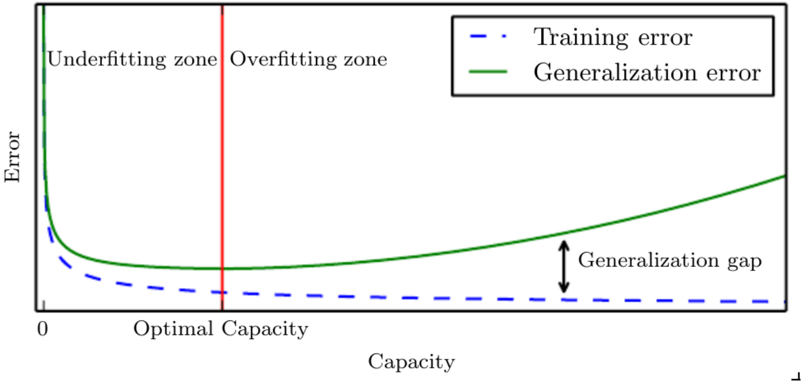

- As capacity increases, training error decreases
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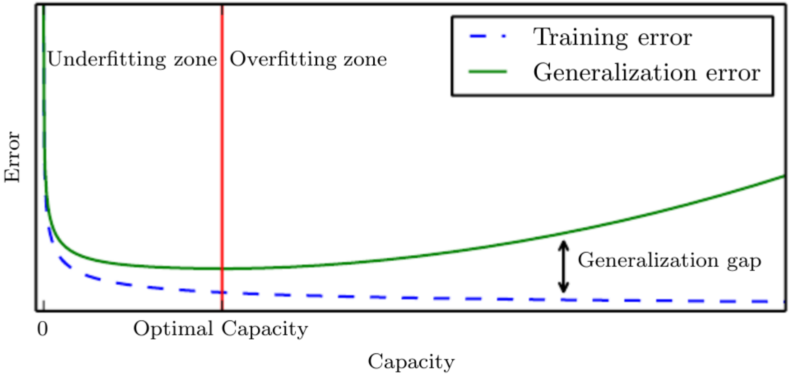

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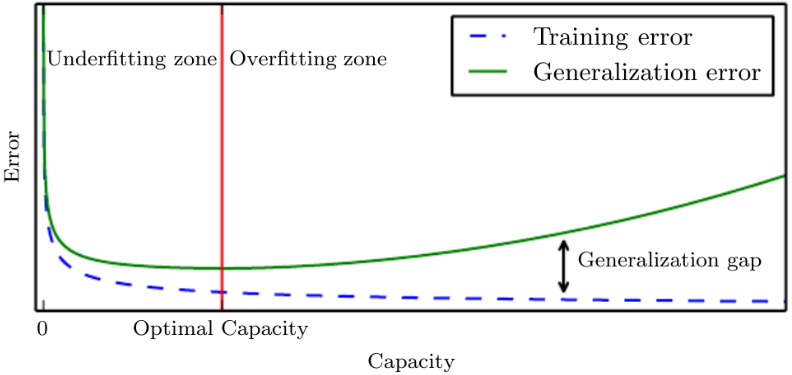

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- Initially, generalization error also decreases
- At some point, generalization error starts increasing
- Optimum capacity is not where training error is minimum

Theory and practice

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- Add a penalty for model complexity to the loss function
- Trade off lower training error against penalty

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Hyperparameters

- Settings that adjust the capacity — e.g., degree of polynomial
- Set externally, not learned
- Search hyperparameter combinations for optimal settings

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- Supervised learning builds a model that minimize training error
- Real goal is to minimize generalization error
- PAC learning provides a theoretical framework to justify this
- Discrepancies in representational capacity of models can cause underfitting or overfitting
- In practice, use regularization and hyperparameter search to identify optimum capacity