Lecture 1: Theoretical foundations of ML

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Advanced Machine Learning
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Supervised learning

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  - 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
  - Choose M to minimize error (loss) with respect to this set
  - Why should M generalize well to arbitrary data?

No free lunch

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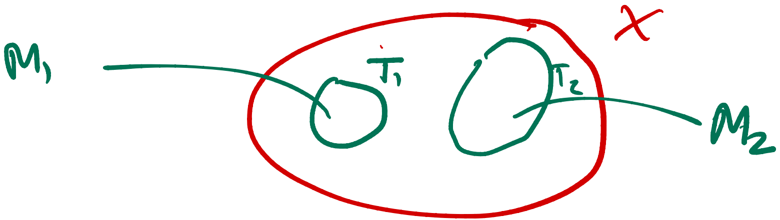
No Free Lunch Theorem [Wolpert, Macready 1997]

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



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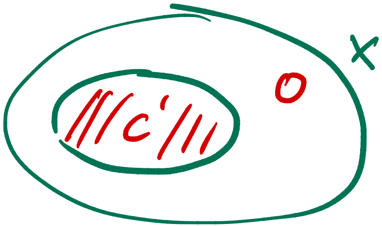
  - e.g., X is all emails, C is the set of spam emails



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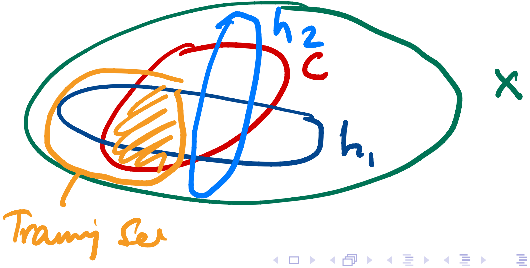

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  - $\text{err}_D(h) = \text{Prob}(h \Delta C)$
  - $h \Delta C = (h \setminus C) \cup (C \setminus h)$ is the symmetric difference

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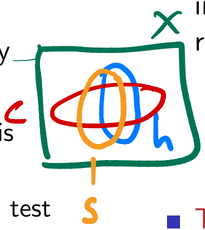

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  - $h \Delta C = (h \setminus C) \cup (C \setminus h)$ is the symmetric difference
- Training error: Given a (finite) training sample $S \subseteq X$
  - $\text{err}_S(h) = |S \cap (h \Delta C)|/|S|$

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- Overfitting Low training error but high true error
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- 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

- Assume $\mathcal{H}$ is finite — use $|\mathcal{H}|$ for capacity

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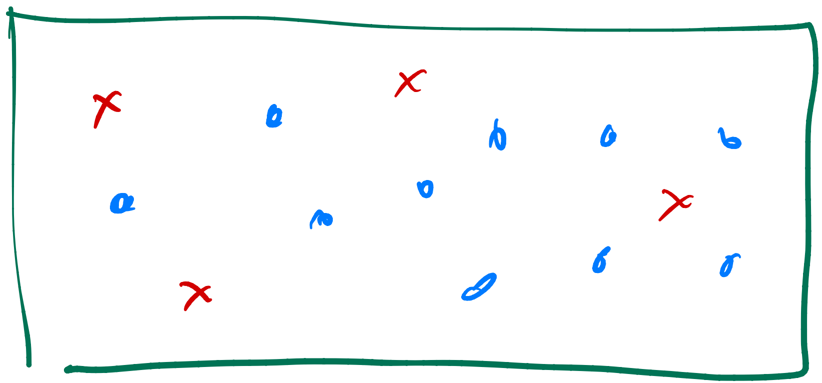
Theorem (PAC learning guarantee)

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



Small Samples

All red

All blue

Big samples

All red is hard

$|S| > 4$

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 $|\text{err}_S(h) - \text{err}_D(h)| \leq \epsilon$.

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

Optimize within training set

Probably Approximately Correct (PAC) learning

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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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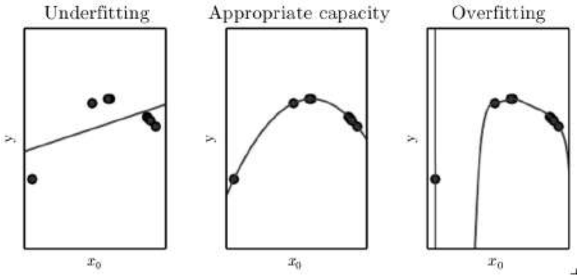

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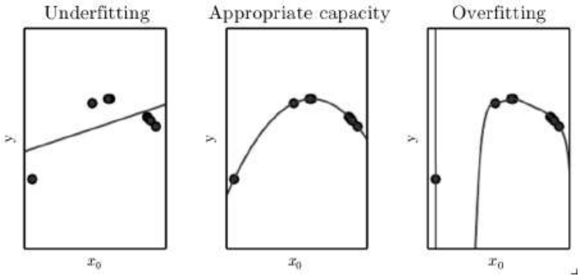

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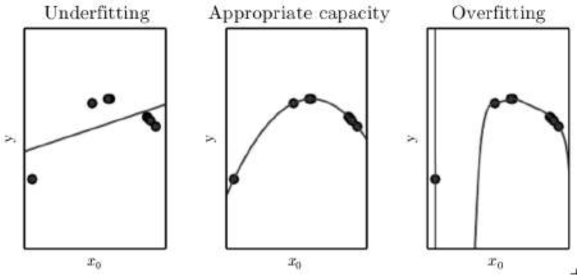

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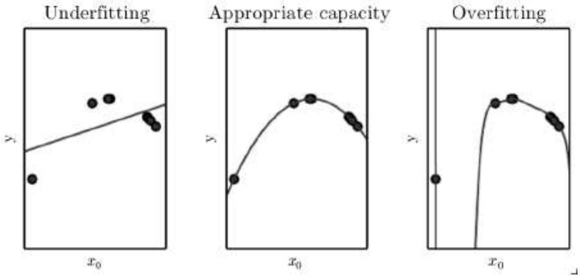

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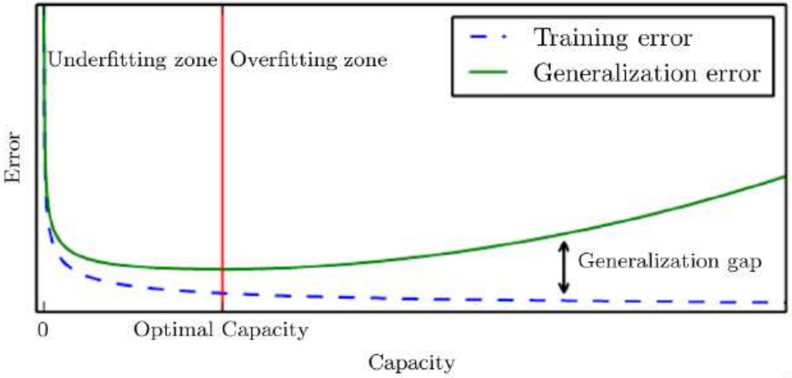
Capacity and error



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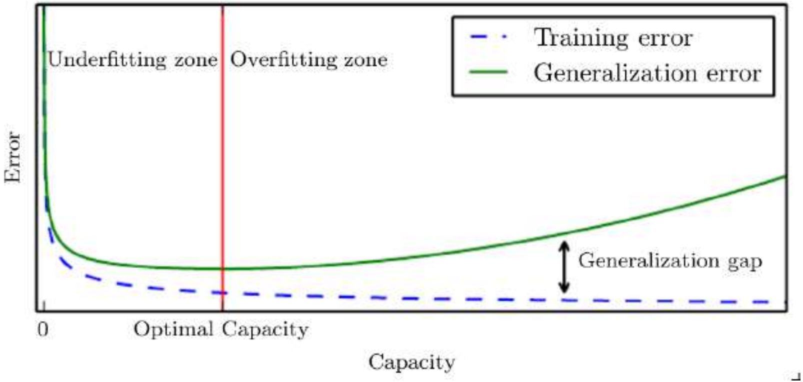

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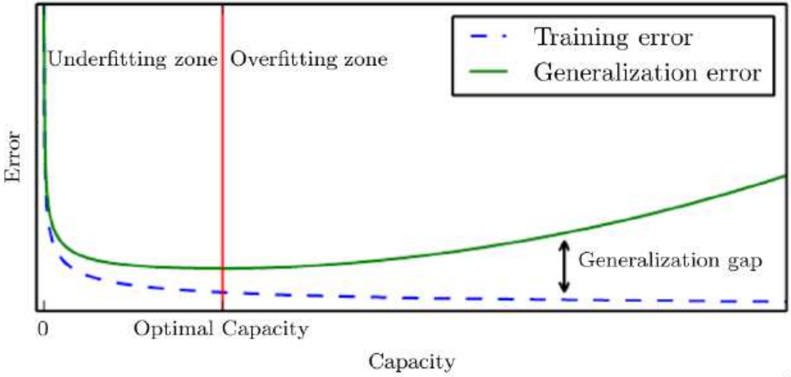

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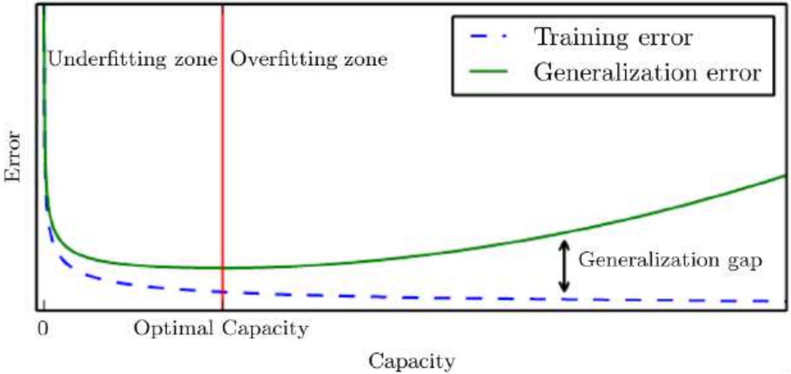

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- Optimum capacity is not where training error is minimum

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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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- 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