What is Machine Learning?

- Definition:
  - A computer program is said to **learn** from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

[T Mitchell, 1997]

Inductive learning (aka concept learning)

- Induction:
  - Given a training set of examples of the form (x,f(x))
    - x is the input, f(x) is the output
  - Return a function h that approximates f
    - h is called the hypothesis

Classification

- Training set:

Sky	Humidity	Wind	Water	Forecast	EnjoySport
Sunny	Normal	Strong	Warm	Same	Yes
Sunny	High	Strong	Warm	Same	Yes
Sunny	High	Strong	Warm	Change	No
Sunny	High	Strong	Cool	Change	Yes

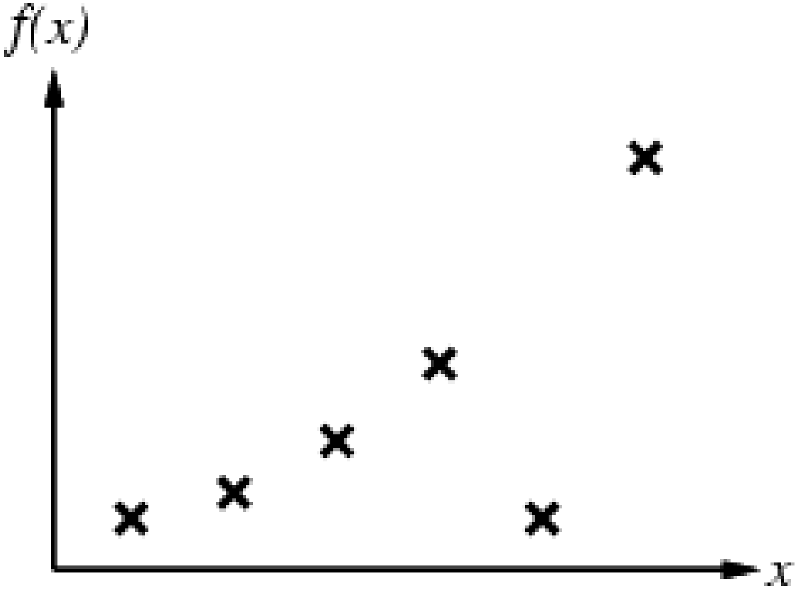
x

f(x)

- Possible hypotheses:
  - h_1: S=sunny → ES=yes
  - h_2: Wa=cool or F=same → enjoySport

Regression

- Find function **h** that fits f at instances x



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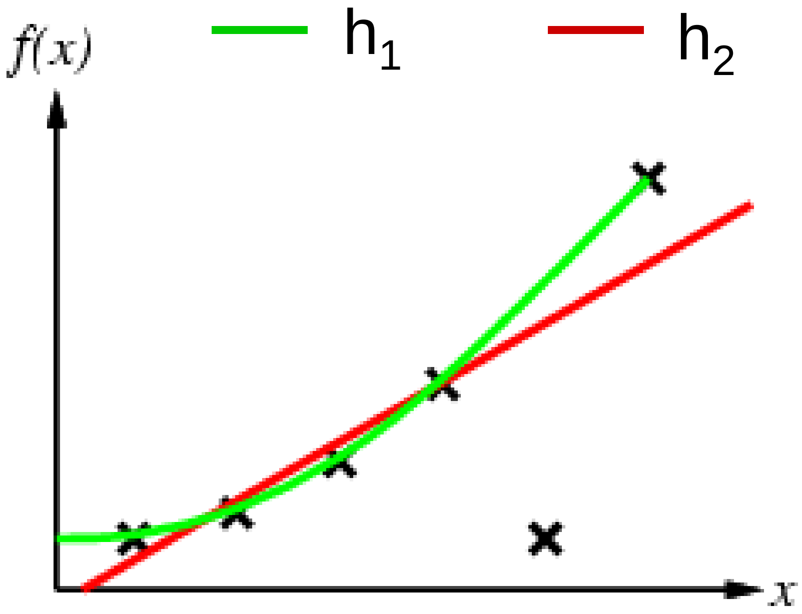


Hypothesis Space

- Hypothesis space H
  - Set of all hypotheses h that the learner may consider
  - Learning is a search through hypothesis space
- Objective:
  - Find hypothesis that agrees with training examples
  - But what about unseen examples?

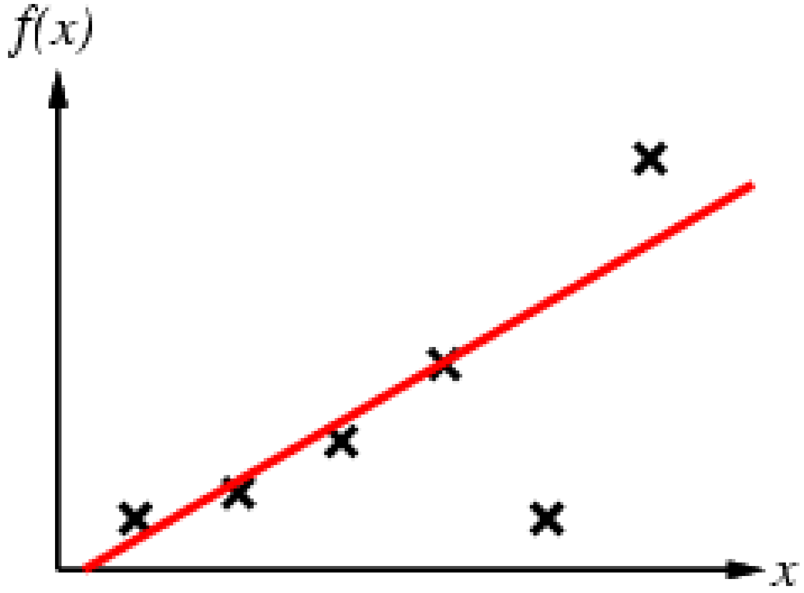
Generalization

- A good hypothesis will generalize well (i.e. predict unseen examples correctly)

- Usually…
  - Any hypothesis h found to approximate the target function f well over a sufficiently large set of training examples will also approximate the target function well over any unobserved examples

Inductive learning

- Construct/adjust *h* to agree with *f* on training set
- (*h* is consistent if it agrees with *f* on all examples)
- E.g., curve fitting:



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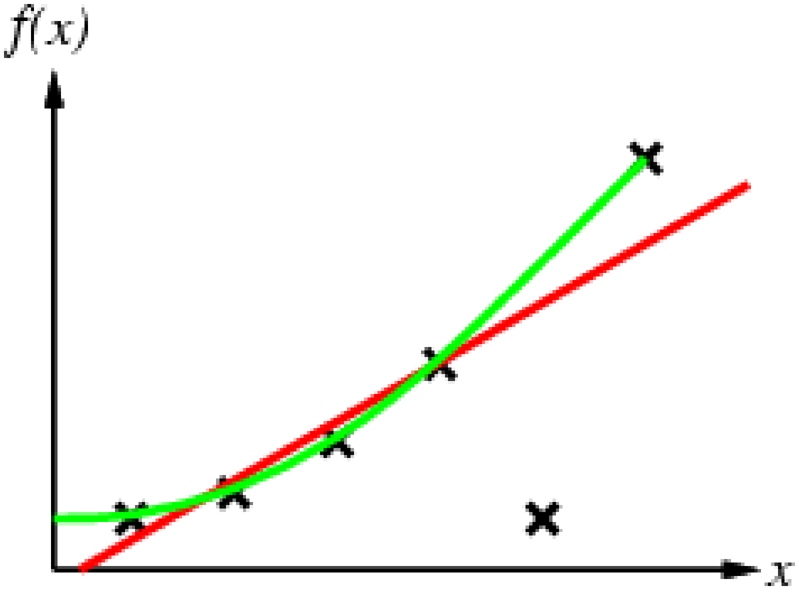

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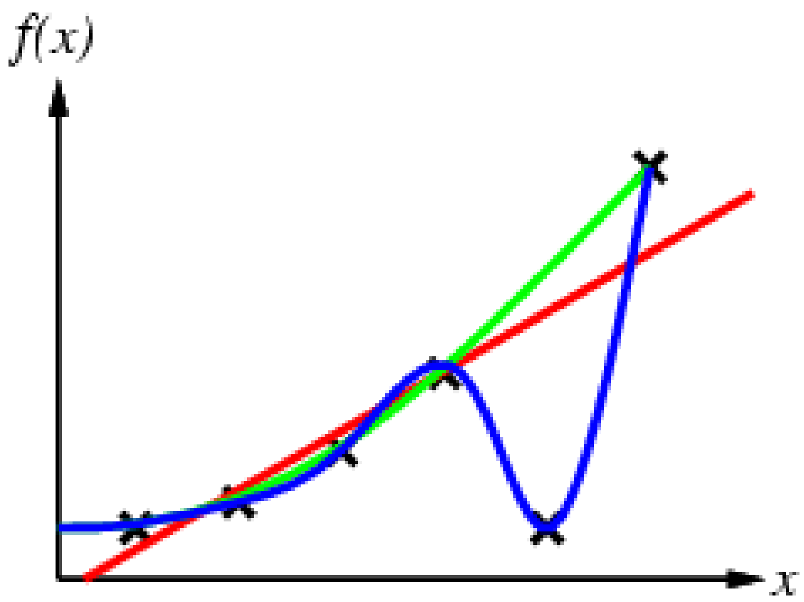

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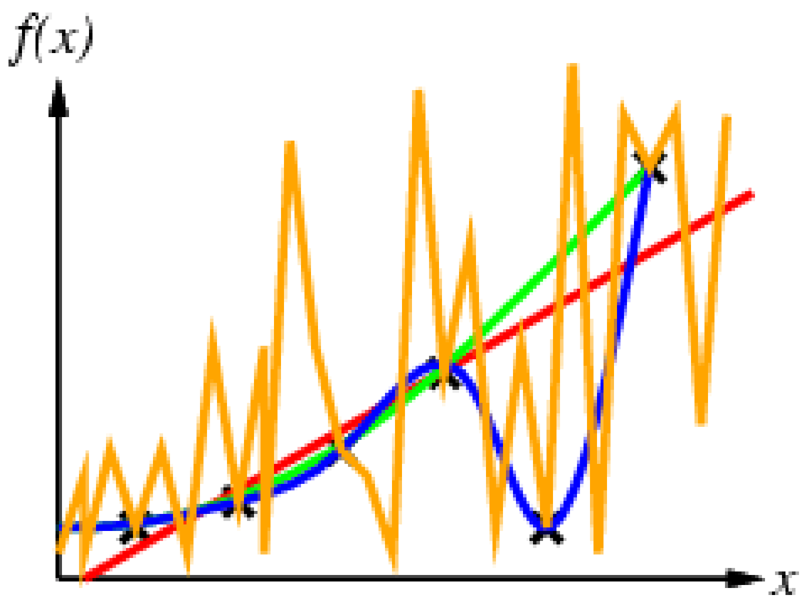

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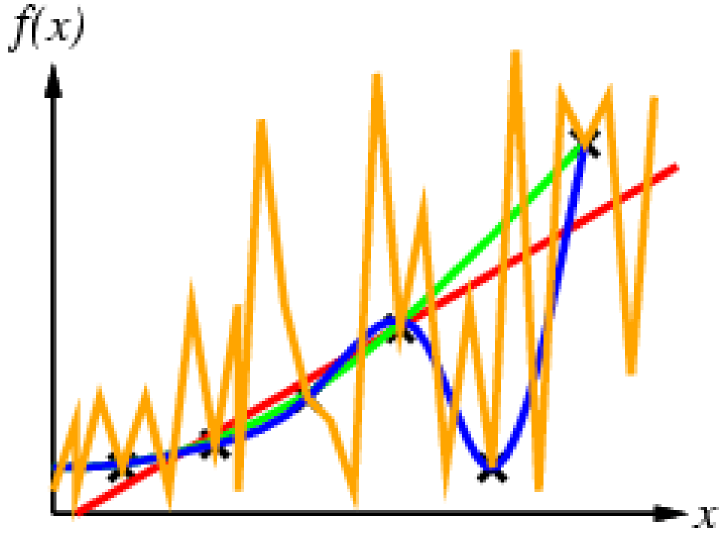


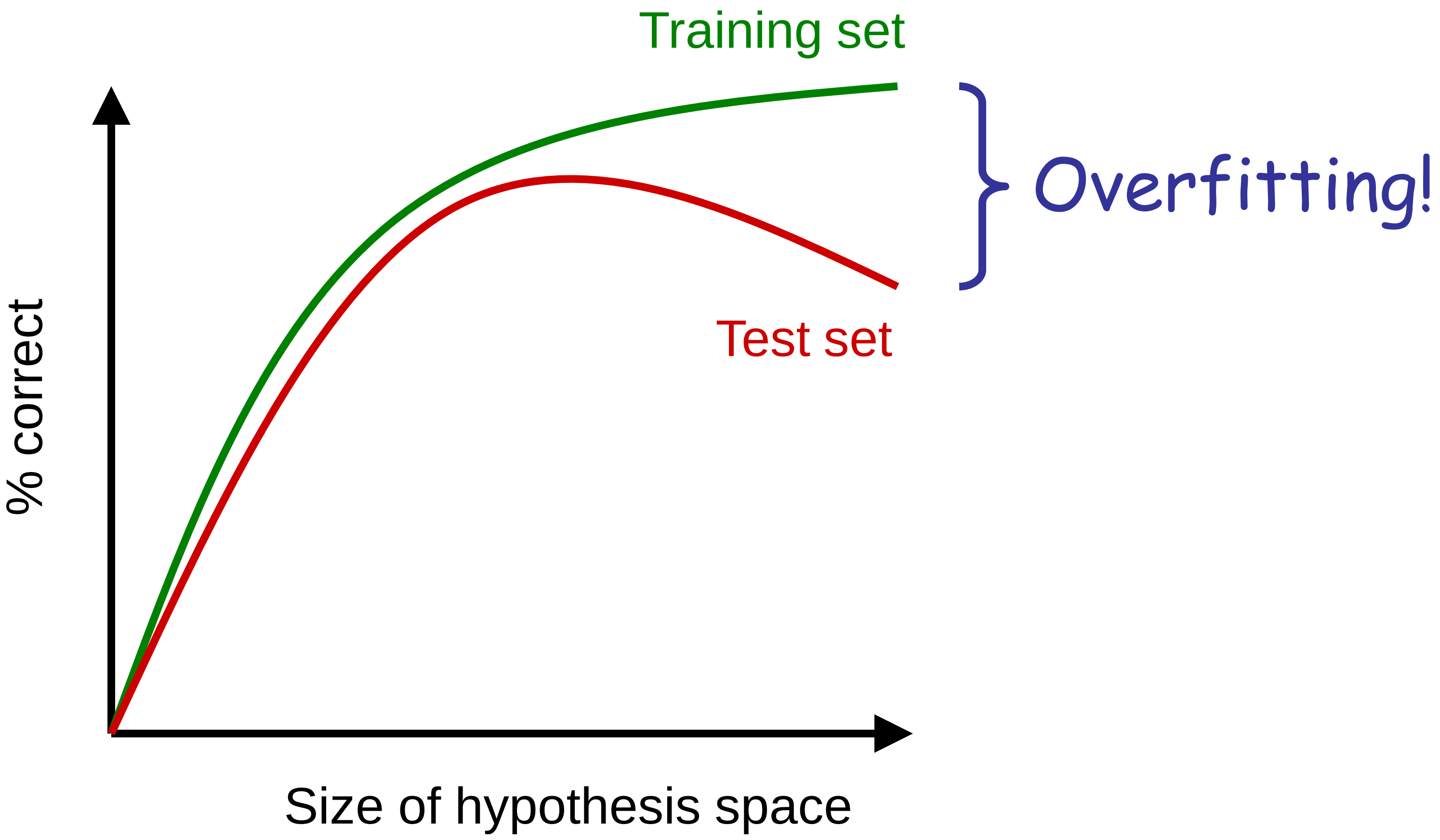
- Ockham's razor: prefer the simplest hypothesis consistent with data

Performance of a learning algorithm

- A learning algorithm is good if it produces a hypothesis that does a good job of predicting classifications of unseen examples

- Verify performance with a **test set**
  1. Collect a large set of examples
  2. Divide into 2 disjoint sets: training set and test set
  3. Learn hypothesis h with training set
  4. Measure percentage of correctly classified examples by h in the test set
  5. Repeat 2-4 for different randomly selected training sets of varying sizes

Learning curves



Overfitting

- **Definition**: Given a hypothesis space H, a hypothesis h ∈ H is said to overfit the training data if there exists some alternative hypothesis h' ∈ H such that h has smaller error than h' over the training examples but h' has smaller error than h over the entire distribution of instances

- Overfitting has been found to decrease accuracy of many algorithms by 10-25%

Statistical Learning

- View: we have uncertain knowledge of the world
- Idea: learning simply reduces this uncertainty

Candy Example

- Favorite candy sold in two flavors:
  - Lime (hugh)
  - Cherry (yum)
- Same wrapper for both flavors
- Sold in bags with different ratios:
  - 100% cherry
  - 75% cherry + 25% lime
  - 50% cherry + 50% lime
  - 25% cherry + 75% lime
  - 100% lime

Candy Example

- You bought a bag of candy but don't know its flavor ratio
- After eating k candies:
  - What's the flavor ratio of the bag?
  - What will be the flavor of the next candy?

Statistical Learning

- Hypothesis H: probabilistic theory of the world
  - h_1: 100% cherry
  - h_2: 75% cherry + 25% lime
  - h_3: 50% cherry + 50% lime
  - h_4: 25% cherry + 75% lime
  - h_5: 100% lime
- Data D: evidence about the world
  - d_1: 1st candy is cherry
  - d_2: 2nd candy is lime
  - d_3: 3rd candy is lime
  - …

Bayesian Learning

- Prior: Pr(H)
- Likelihood: Pr(d|H)
- Evidence: $\mathbf{d} = \langle d_1, d_2, \ldots, d_n \rangle$

- Bayesian Learning amounts to computing the posterior using Bayes' Theorem:

$$Pr(H|\mathbf{d}) = k\, Pr(\mathbf{d}|H) Pr(H)$$

Bayesian Prediction

- Suppose we want to make a prediction about an unknown quantity X (i.e., the flavor of the next candy)

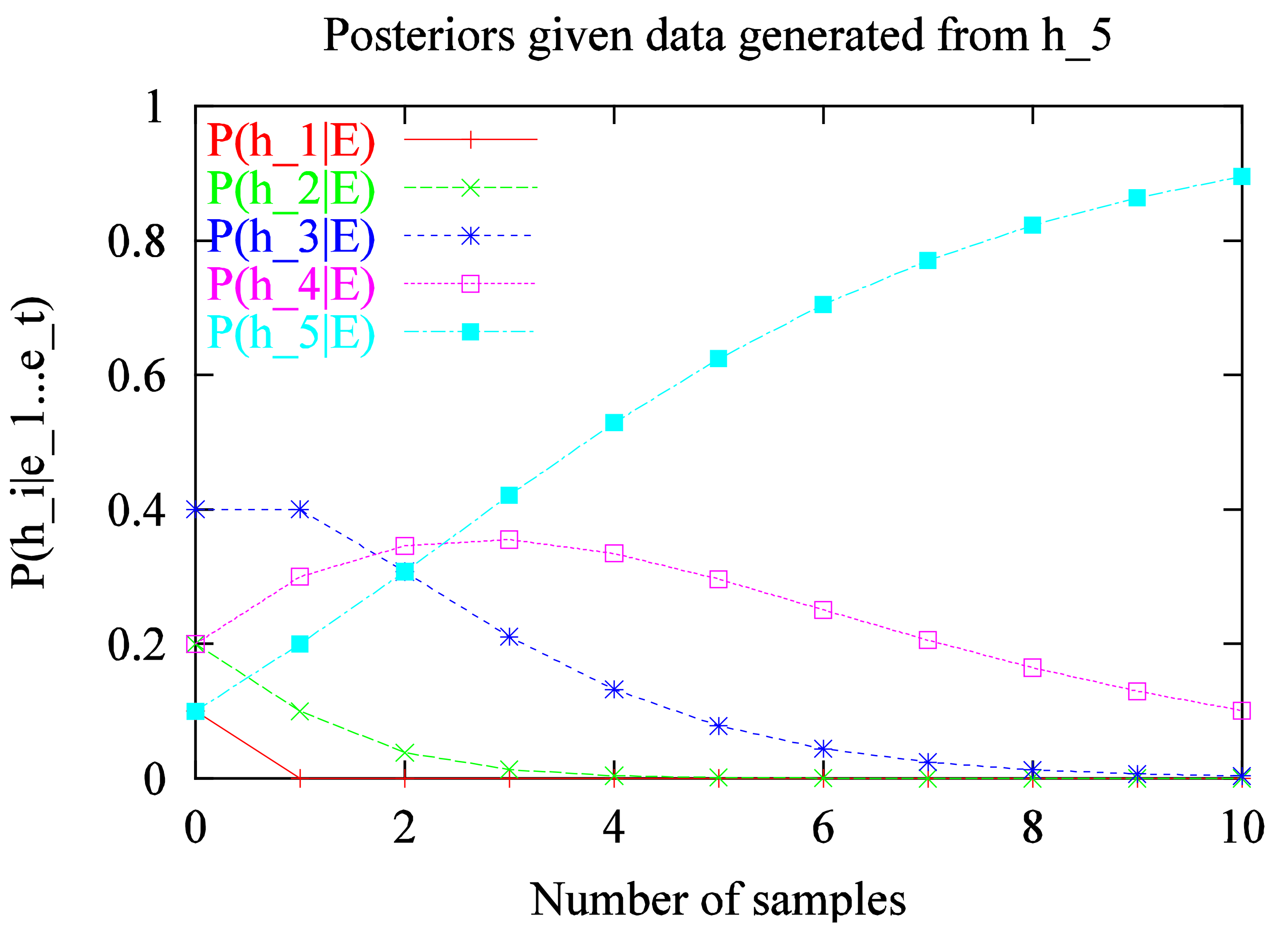
- $Pr(X|\mathbf{d}) = \Sigma_i Pr(X|\mathbf{d},h_i)P(h_i|\mathbf{d})$
  $= \Sigma_i Pr(X|h_i)P(h_i|\mathbf{d})$

- Predictions are weighted averages of the predictions of the individual hypotheses
- Hypotheses serve as "intermediaries" between raw data and prediction

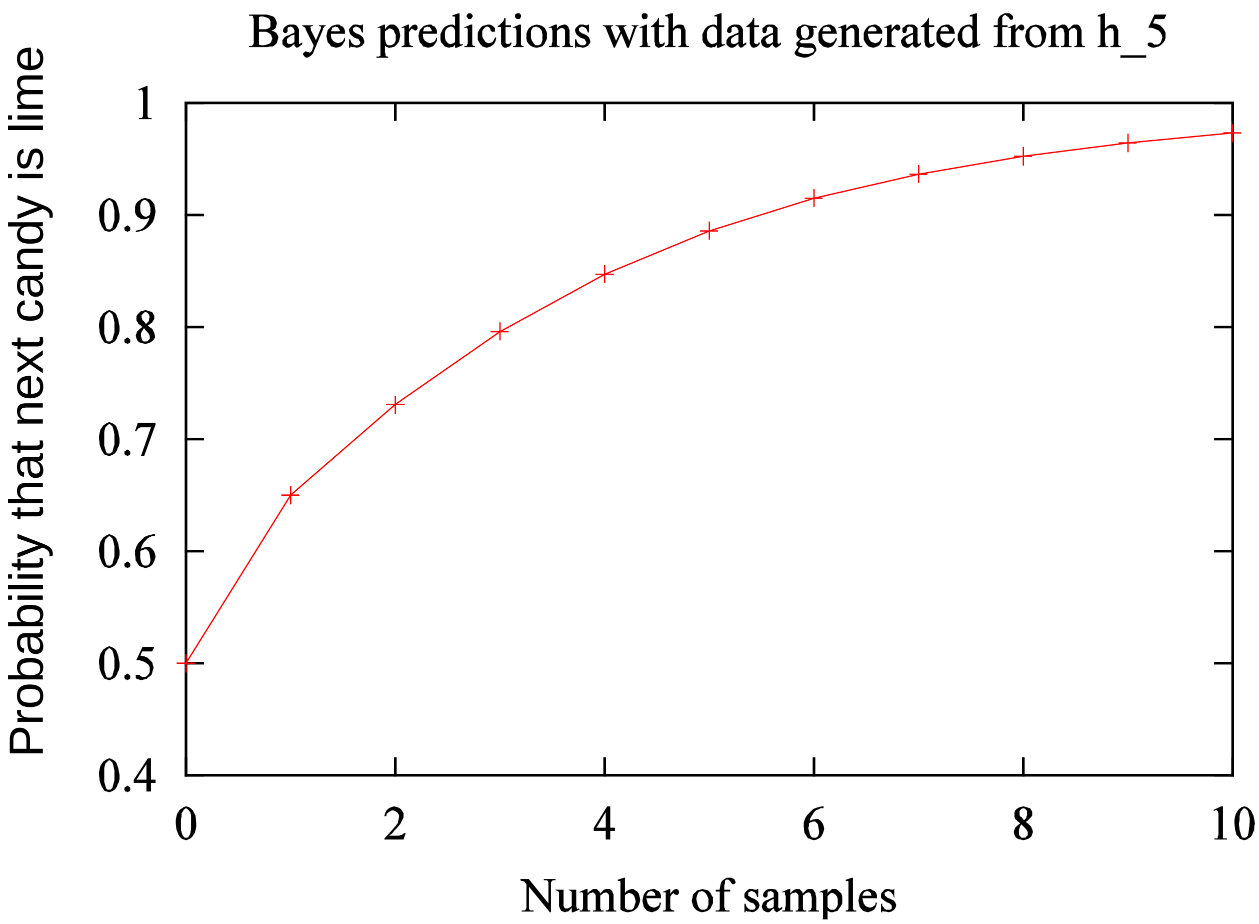
Candy Example

- Assume prior $P(H) = \langle 0.1, 0.2, 0.4, 0.2, 0.1 \rangle$
- Assume candies are i.i.d. (identically and independently distributed)
  - $P(\mathbf{d}|h) = \Pi_j P(d_j|h)$
- Suppose first 10 candies all taste lime:
  - $P(\mathbf{d}|h_5) = 1^{10} = 1$
  - $P(\mathbf{d}|h_3) = 0.5^{10} = 0.00097$
  - $P(\mathbf{d}|h_1) = 0^{10} = 0$

Posterior


Posteriors given data generated from h_5
P(h_1|E)
P(h_2|E)
P(h_3|E)
P(h_4|E)
P(h_5|E)
P(h_i|e_1...e_t)
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
10
Number of samples

Prediction



Bayes predictions with data generated from h_5
Probability that next candy is lime
1
0.9
0.8
0.7
0.6
0.5
0.4
0
2
4
6
8
10
Number of samples

Bayesian Learning

- Bayesian learning properties:
  - **Optimal** (i.e. given prior, no other prediction is correct more often than the Bayesian one)
  - **No overfitting** (prior can be used to penalize complex hypotheses)
- There is a price to pay:
  - When hypothesis space is large Bayesian learning may be intractable
  - i.e. sum (or integral) over hypothesis often intractable
- Solution: approximate Bayesian learning

Maximum a posteriori (MAP)

- Idea: make prediction based on most probable hypothesis h_{MAP}
  - $h_{MAP} = \text{argmax}_{h_i} P(h_i|\mathbf{d})$
  - $P(X|\mathbf{d}) \approx P(X|h_{MAP})$

- In contrast, Bayesian learning makes prediction based on **all** hypotheses weighted by their probability

Candy Example (MAP)

- Prediction after
  - 1 lime: $h_{MAP} = h_3$, $Pr(lime|h_{MAP}) = 0.5$
  - 2 limes: $h_{MAP} = h_4$, $Pr(lime|h_{MAP}) = 0.75$
  - 3 limes: $h_{MAP} = h_5$, $Pr(lime|h_{MAP}) = 1$
  - 4 limes: $h_{MAP} = h_5$, $Pr(lime|h_{MAP}) = 1$
  - …

- After only 3 limes, it correctly selects h_5

Candy Example (MAP)

- But what if correct hypothesis is h_4?
  - h_4: P(lime) = 0.75 and P(cherry) = 0.25

- After 3 limes
  - MAP incorrectly predicts h_5
  - MAP yields $P(lime|h_{MAP}) = 1$
  - Bayesian learning yields $P(lime|\mathbf{d}) = 0.8$

MAP properties

- MAP prediction **less accurate** than Bayesian prediction since it relies only on **one** hypothesis h_{MAP}
- But MAP and Bayesian predictions converge as data increases
- No overfitting (prior can be used to penalize complex hypotheses)
- Finding h_{MAP} may be intractable:
  - $h_{MAP} = \text{argmax } P(h|\mathbf{d})$
  - Optimization may be difficult

MAP computation

- Optimization:
  - $h_{MAP} = \text{argmax}_h \, P(h|\mathbf{d})$
    $= \text{argmax}_h \, P(h) \, P(\mathbf{d}|h)$
    $= \text{argmax}_h \, P(h) \, \Pi_i \, P(d_i|h)$

- Product induces non-linear optimization
- Take the log to linearize optimization
  - $h_{MAP} = \text{argmax}_h \log P(h) + \Sigma_i \log P(d_i|h)$

Maximum Likelihood (ML)

- Idea: simplify MAP by assuming uniform prior (i.e., $P(h_i) = P(h_j)\ \forall i,j$)
  - $h_{MAP} = \text{argmax}_h\ P(h)\ P(\mathbf{d}|h)$
  - $h_{ML} = \text{argmax}_h\ P(\mathbf{d}|h)$

- Make prediction based on h_{ML} only:
  - $P(X|\mathbf{d}) \approx P(X|h_{ML})$

Candy Example (ML)

- Prediction after
  - 1 lime: $h_{ML} = h_5$, $Pr(lime|h_{ML}) = 1$
  - 2 limes: $h_{ML} = h_5$, $Pr(lime|h_{ML}) = 1$
  - …
- Frequentist: "objective" prediction since it relies only on the data (i.e., no prior)
- Bayesian: prediction based on data and uniform prior (since no prior ≡ uniform prior)

ML properties

- ML prediction **less accurate** than Bayesian and MAP predictions since it ignores prior info and relies only on **one** hypothesis h_{ML}
- But ML, MAP and Bayesian predictions converge as data increases
- Subject to overfitting (no prior to penalize complex hypothesis that could exploit statistically insignificant data patterns)

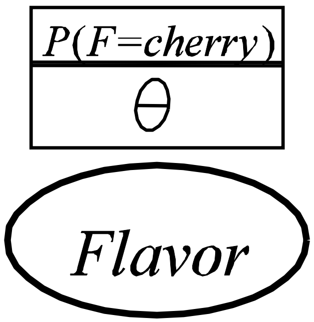
- Finding h_{ML} is often easier than h_{MAP}
  - $h_{ML} = \text{argmax}_h \sum_i \log P(d_i|h)$

Statistical Learning

- Use Bayesian Learning, MAP or ML
- Complete data:
  - When data has multiple attributes, **all attributes are known**
  - Easy
- Incomplete data:
  - When data has multiple attributes, **some attributes are unknown**
  - Harder

Simple ML example

- Hypothesis h_θ:
  - P(cherry)=θ & P(lime)=1-θ
- Data **d**:
  - c cherries and l limes



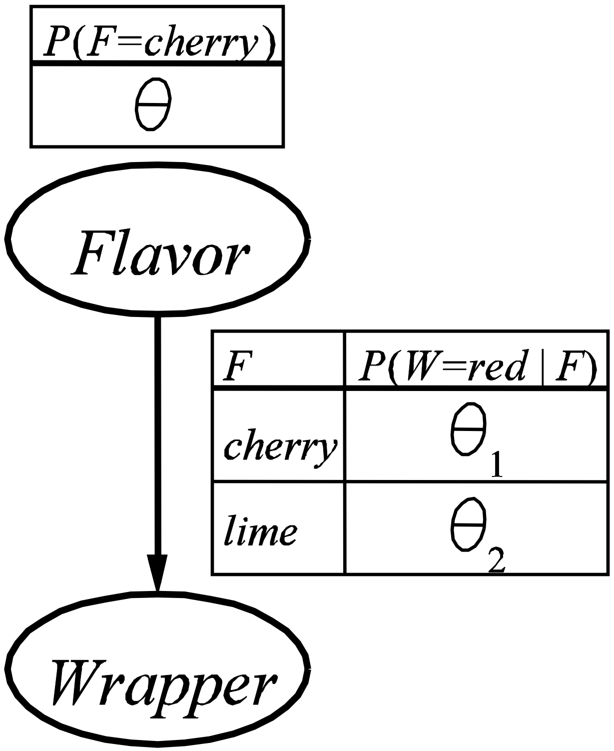
- ML hypothesis:
  - θ is relative frequency of observed data
  - θ = c/(c+l)
  - P(cherry) = c/(c+l) and P(lime)= l/(c+l)

ML computation

- 1) Likelihood expression
  - $P(\mathbf{d}|h_\theta) = \theta^c (1-\theta)^l$
- 2) log likelihood
  - $\log P(\mathbf{d}|h_\theta) = c \log \theta + l \log (1-\theta)$
- 3) log likelihood derivative
  - $d(\log P(\mathbf{d}|h_\theta))/d\theta = c/\theta - l/(1-\theta)$
- 4) ML hypothesis
  - $c/\theta - l/(1-\theta) = 0 \rightarrow \theta = c/(c+l)$

More complicated ML example

- Hypothesis: $h_{\theta,\theta_1,\theta_2}$
- Data:
  - c cherries
    - g_c green wrappers
    - r_c red wrappers
  - l limes
    - g_l green wrappers
    - r_l red wrappers

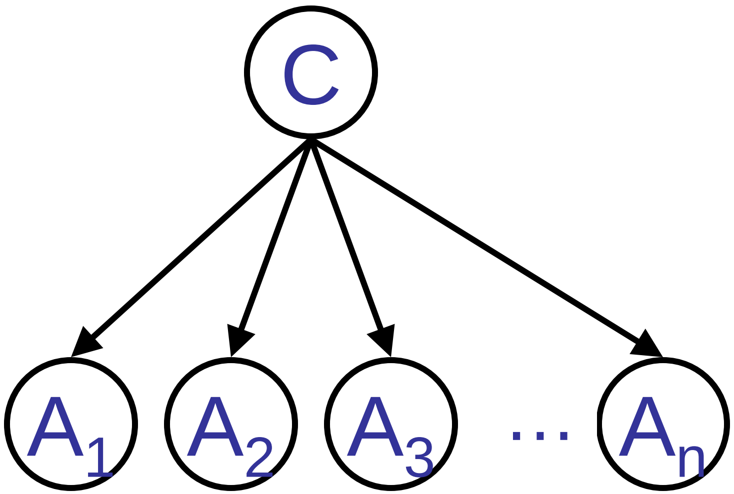


ML computation

- 1) Likelihood expression
  - $P(\mathbf{d}|h_{\theta,\theta_1,\theta_2}) = \theta^c(1-\theta)^l \; \theta_1^{r_c}(1-\theta_1)^{g_c} \; \theta_2^{r_l}(1-\theta_2)^{g_l}$
- ...
- 4) ML hypothesis
  - $c/\theta - l/(1-\theta) = 0 \rightarrow \theta = c/(c+l)$
  - $r_c/\theta_1 - g_c/(1-\theta_1) = 0 \rightarrow \theta_1 = r_c/(r_c+g_c)$
  - $r_l/\theta_2 - g_l/(1-\theta_2) = 0 \rightarrow \theta_2 = r_l/(r_l+g_l)$

Naïve Bayes model

- Want to predict a class C based on attributes A_i
- Parameters:
  - $\theta = P(C{=}true)$
  - $\theta_{i1} = P(A_i{=}true|C{=}true)$
  - $\theta_{i2} = P(A_i{=}true|C{=}false)$
- Assumption: A_i's are independent given C



Naïve Bayes model for Restaurant Problem

- Data:

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

- ML sets
  - θ to relative frequencies of *wait* and *~wait*
  - θ_{i1}, θ_{i2} to relative frequencies of each attribute value given *wait* and *~wait*