Statistical learning

Chapter 20 (plus 18.1-2)

Outline

- ♢ Forms of Learning
- ♢ Bayesian learning
- ♢ Maximum likelihood and linear regression
- ♢ Expectation Maximization

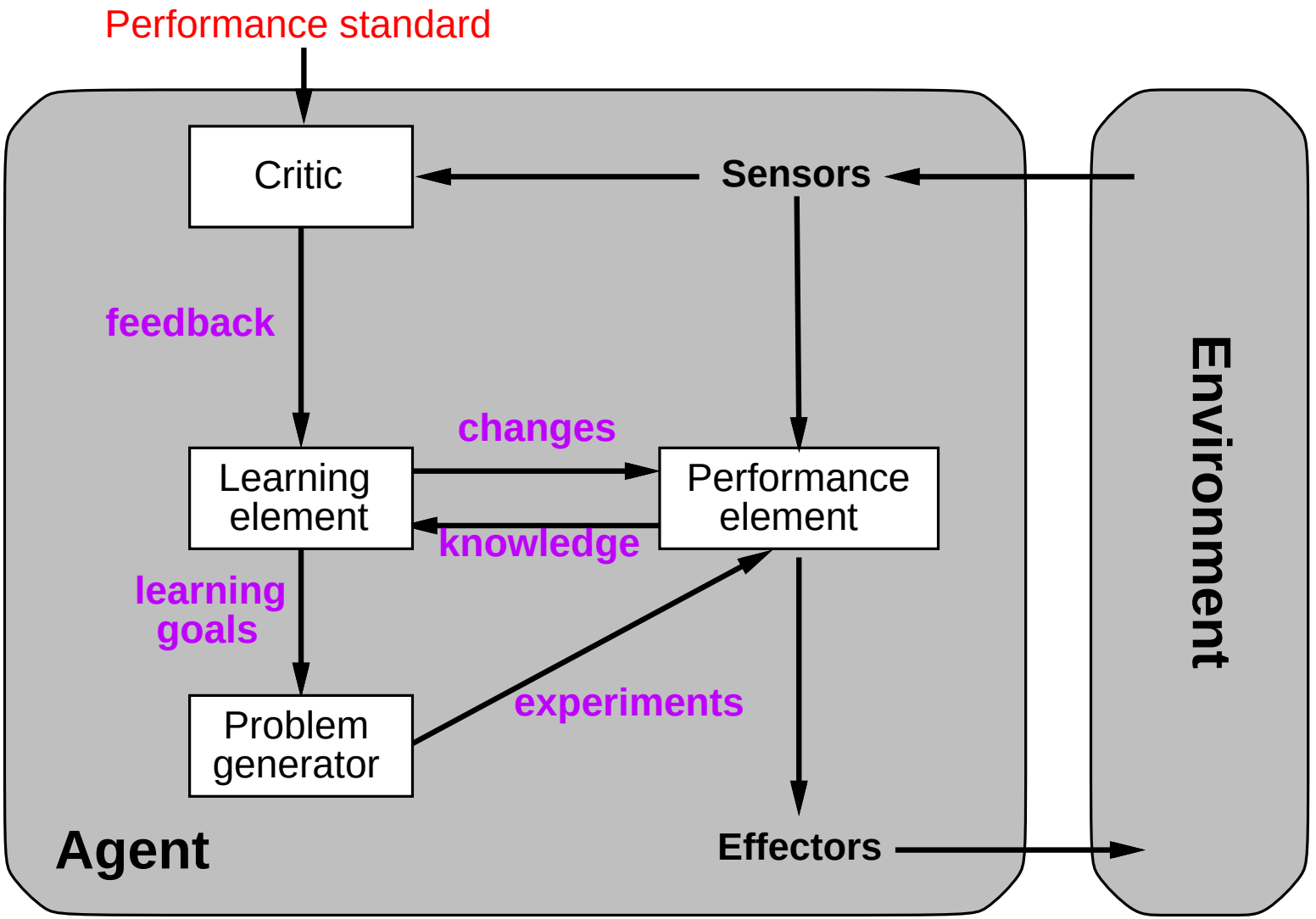
Learning

Learning is essential for unknown environments,
i.e., when designer lacks omniscience

Learning is useful as a system construction method,
i.e., expose the agent to reality rather than trying to write it down

Learning modifies the agent's decision mechanisms to improve performance

Learning agents



Learning element

Design of learning element is dictated by

- ♢ what type of performance element is used
- ♢ which functional component is to be learned
- ♢ how that functional component is represented
- ♢ what kind of feedback is available

Example scenarios:

Performance element	Component	Representation	Feedback
Alpha–beta search	Eval. fn.	Weighted linear function	Win/loss
Logical agent	Transition model	Successor–state axioms	Outcome
Utility–based agent	Transition model	Dynamic Bayes net	Outcome
Simple reflex agent	Percept–action fn	Neural net	Correct action

Types of learning

Supervised learning: learn a function from examples labeled with the correct answers (requires "teacher")

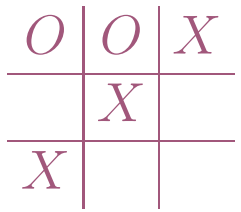
Unsupervised learning: learn patterns in the input when no specific output (or answers) are given (no "teacher")

Reinforcement learning: learn from occasional rewards (harder, but does not require a teacher)

Inductive learning (a.k.a. Science)

Simplest form: learn a function from examples (**tabula rasa**)

f is the target function

An example is a pair x, $f(x)$, e.g.,  , $+1$

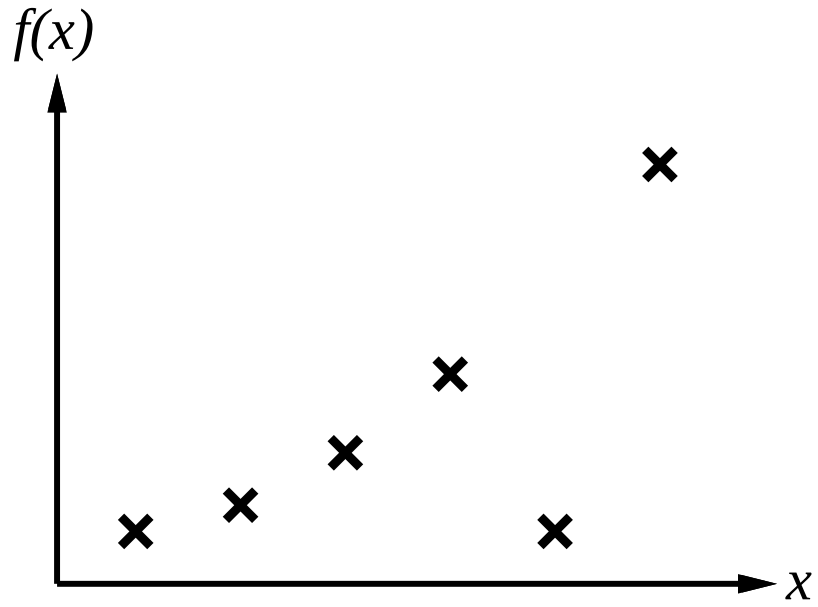
Problem: find a(n) hypothesis h
such that $h \approx f$
given a training set of examples

(This is a highly simplified model of real learning:
- **Ignores prior knowledge**
- **Assumes a deterministic, observable "environment"**
- **Assumes examples are given**
- **Assumes that the agent wants to learn f—why?)**

Inductive learning method

Construct/adjust h to agree with f on training set
(h is consistent if it agrees with f on all examples)

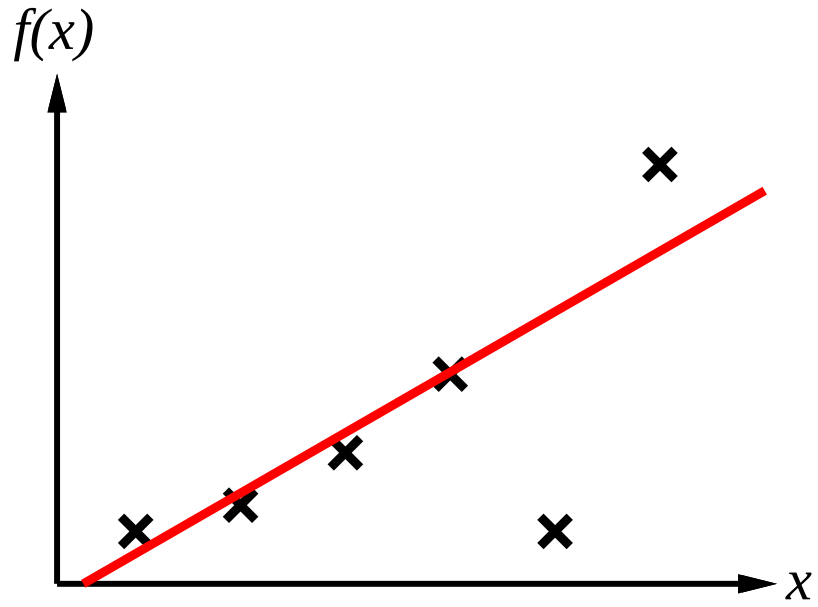
E.g., curve fitting:



Inductive learning method

Construct/adjust h to agree with f on training set
(h is consistent if it agrees with f on all examples)

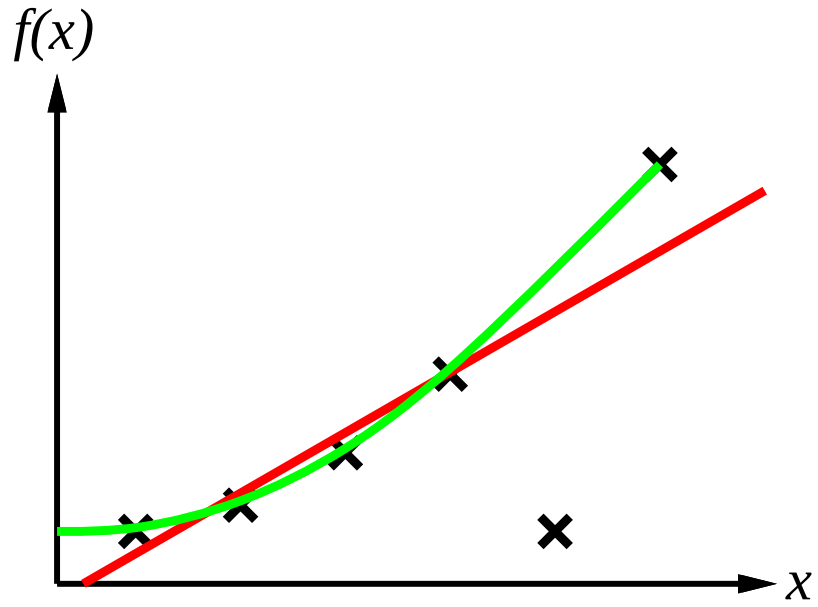
E.g., curve fitting:



Inductive learning method

Construct/adjust h to agree with f on training set
(h is consistent if it agrees with f on all examples)

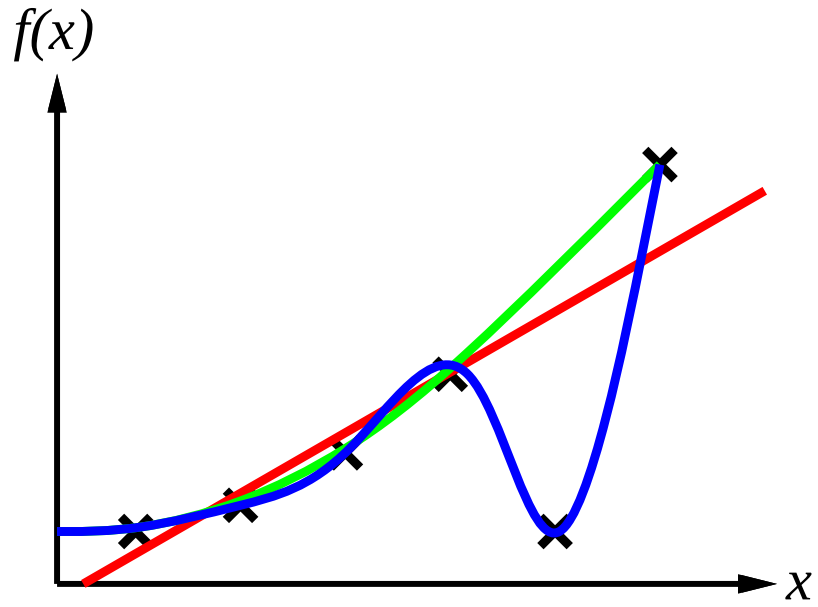
E.g., curve fitting:



Inductive learning method

Construct/adjust h to agree with f on training set
(h is consistent if it agrees with f on all examples)

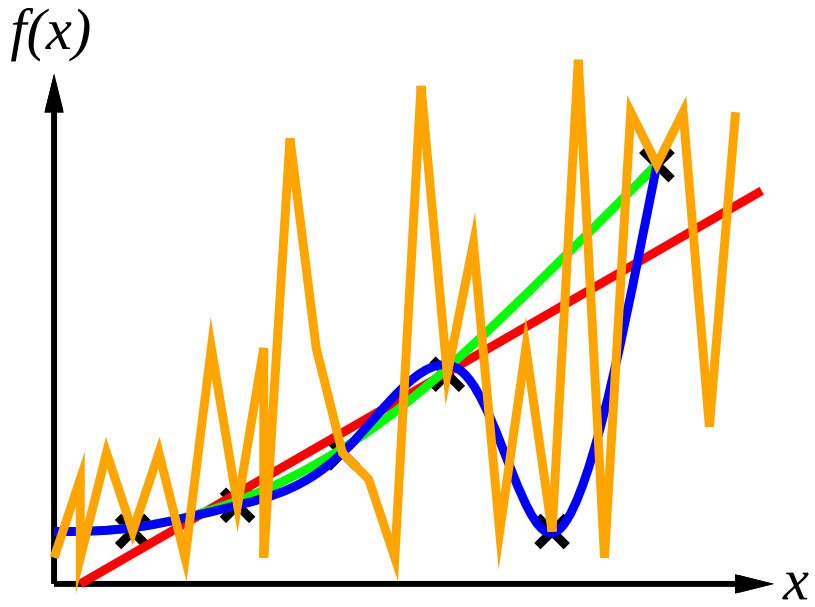
E.g., curve fitting:



Inductive learning method

Construct/adjust h to agree with f on training set
(h is consistent if it agrees with f on all examples)

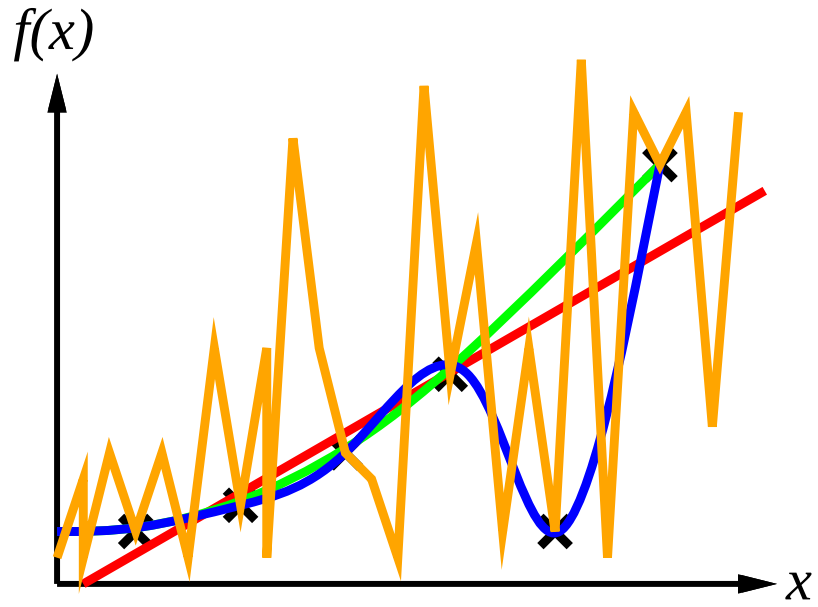
E.g., curve fitting:



Inductive learning method

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:



Ockham's razor: maximize a combination of consistency and simplicity

Moving on to: Statistical learning

Chapter 20

Full Bayesian learning

(This is a form of unsupervised learning.)

View learning as Bayesian updating of probability distribution
over the hypothesis space

Prior $\mathbf{P}(H)$, data evidence given as $\mathbf{d} = d_1, \ldots, d_N$

Given the data so far, each hypothesis has a posterior probability:

$$P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$$

Predictions use a likelihood-weighted average over the hypotheses:

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

Assume observations are independently and identically distributed (i.e., i.i.d):

$$\mathbf{P}(\mathbf{d}|h_i) = \Pi_j \, P(d_j|h_i)$$

Example

Suppose there are five kinds of bags of candies:

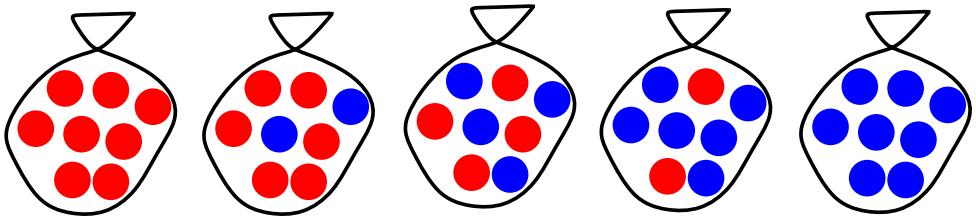
10% are h_1: 100% lime candies

20% are h_2: 75% lime candies + 25% cherry candies

40% are h_3: 50% lime candies + 50% cherry candies

20% are h_4: 25% lime candies + 75% cherry candies

10% are h_5: 100% cherry candies



Then we observe candies drawn from some bag: 

What kind of bag is it? What flavor will the next candy be?

Posterior probability of hypotheses

For example, since here we have 10 cherry candies in a row, the likelihood that this was generated by a given hypothesis is:

$$P(\mathbf{d}|h_1) = 0^{10} = 0$$

$$P(\mathbf{d}|h_2) = 0.25^{10} = 0.954 \times 10^{-7}$$

$$P(\mathbf{d}|h_3) = 0.5^{10} = 0.001$$

$$P(\mathbf{d}|h_4) = 0.75^{10} = 0.0563$$

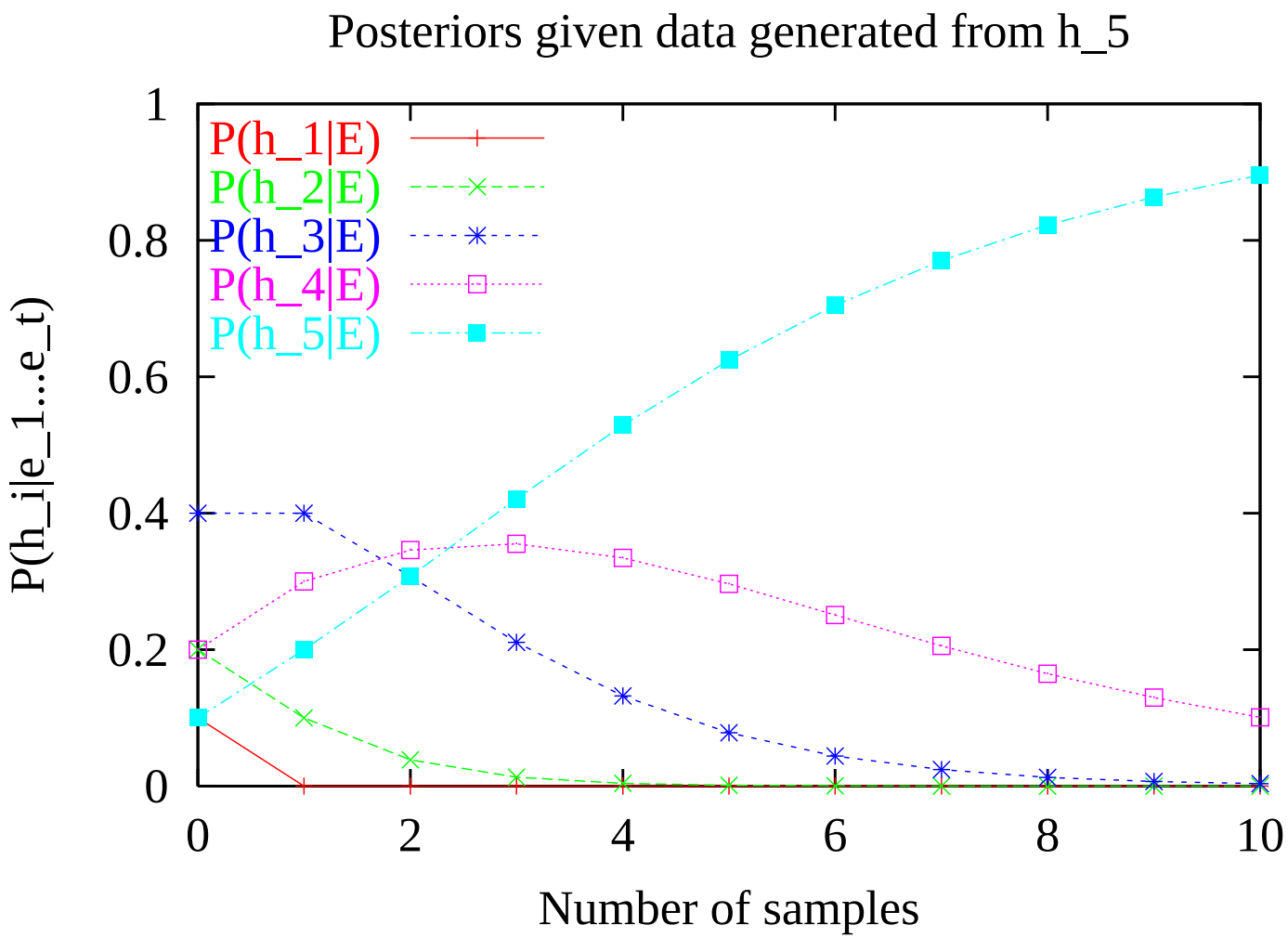
$$P(\mathbf{d}|h_5) = 1^{10} = 1$$

Then, we take into account the prior probabilities of each hypothesis.

Assume that the prior distribution over $h_1, ..., h_5$ (i.e., $P(h_i)$) is given by: $< 0.1, 0.2, 0.4, 0.2, 0.1 >$

Computing $P(\mathbf{d}|h_i)P(h_i)$ and normalizing, we have ...

Posterior probability of hypotheses



Prediction probability

Let's say we now want to know the probability that the next candy is lime, given that we've seen 10 limes so far. Here our unknown quantity, X, is "next candy is lime".

As we've already seen, we calculate predictions using a likelihood-weighted average over the hypotheses:

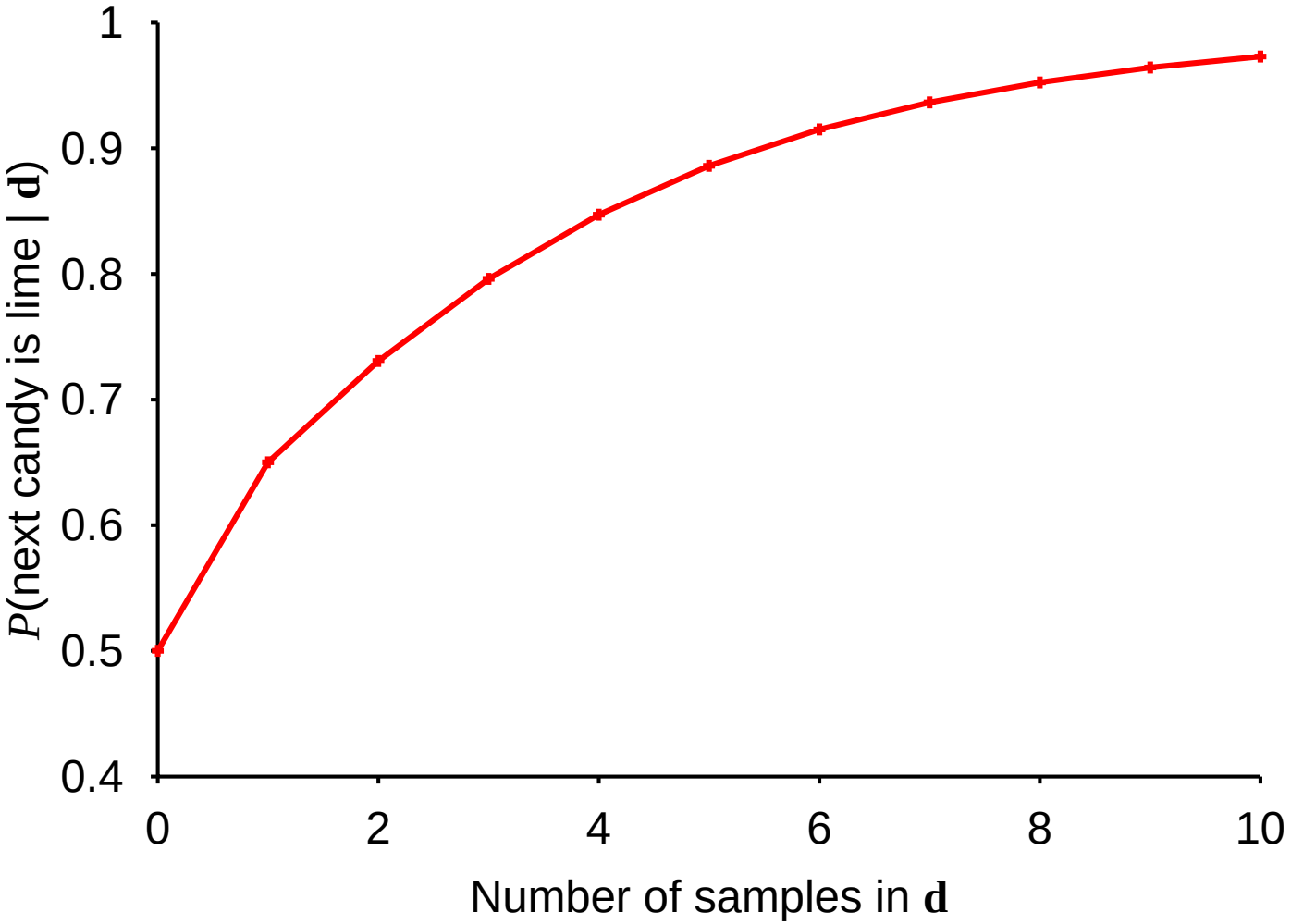
$$\mathbf{P}(X|\mathbf{d}) = \sum_i \mathbf{P}(X|h_i)P(h_i|\mathbf{d})$$

After 10 lime candies, we have:

$$\mathbf{P}(d_{N+1} = lime|d_1...d_N = lime)$$

$$= \sum_i \mathbf{P}(d_{N+1} = lime|h_i)\mathbf{P}(h_i|d_1...d_N = lime)$$

Prediction probability



MAP approximation for predictions

Summing over the hypothesis space is often intractable
(e.g., 18,446,744,073,709,551,616 Boolean functions of 6 attributes)

Maximum a posteriori (MAP) learning: choose h_{MAP} maximizing $P(h_i|\mathbf{d})$

Remember: $P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$

So, maximize $P(\mathbf{d}|h_i)P(h_i)$ or, equivalently,
minimize $-\log P(\mathbf{d}|h_i) - \log P(h_i)$

[By taking logarithms, we reduce the product to a sum over the data, which is usually easier to optimize.]

Log terms can be viewed as:
bits to encode data given hypothesis + bits to encode hypothesis
This is the basic idea of minimum description length (MDL) learning

For deterministic hypotheses, $P(\mathbf{d}|h_i)$ is 1 if consistent, 0 otherwise
$\Rightarrow$ MAP = simplest consistent hypothesis

ML approximation

For large data sets, prior becomes irrelevant

Maximum likelihood (ML) learning: choose h_{ML} maximizing $P(\mathbf{d}|h_i)$

I.e., simply get the best fit to the data; identical to MAP for uniform prior (which is reasonable if all hypotheses are of the same complexity)

ML is the "standard" (non-Bayesian) statistical learning method

Summarizing these 3 types of learning

Bayesian learning:

Calculate $P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$.

MAP (Maximum a posteriori) learning:

Choose h_{MAP} that maximizes $P(\mathbf{d}|h_i)P(h_i)$ or, equivalently, minimizes $-\log P(\mathbf{d}|h_i) - \log P(h_i)$.

(This avoids summing over all hypotheses.)

ML (Maximum likelihood) learning:

Choose h_{ML} maximizing $P(\mathbf{d}|h_i)$.

(This assumes uniform prior for hypotheses, which is reasonable for large data sets.)

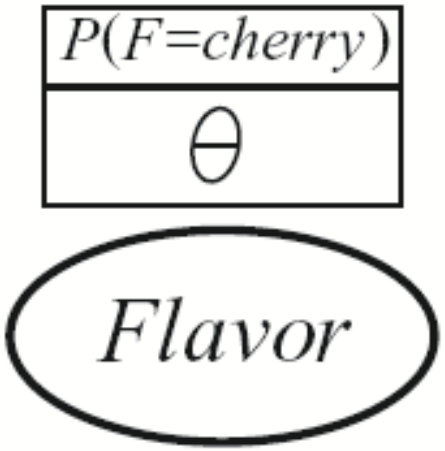
Maximum Likelihood Parameter Learning

Objective: Find numerical parameters for a probability model whose structure is fixed.

Example: A bag of candy

- Unknown fraction of lime/cherry
- Parameter $= \theta =$ proportion of cherry candies
- Hypothesis $= h_\theta =$ proportion of cherry candies
- If assume all proportions are equally likely $a\ priori$, then ML approach is feasible
- If model as Bayesian network, just need one random variable, $Flavor$

Problem Modeled as a Bayesian Network



Example: Bags of Candy

Suppose unwrap N candies, of which c are cherries, and l are limes.

Remember, we have likelihood of data (assuming i.i.d.) is:

$$\mathbf{P}(\mathbf{d}|h_i) = \prod_j P(d_j|h_i)$$

So, $\mathbf{P}(\mathbf{d}|h_\theta) = \prod_{j=1}^{N} P(d_j|h_\theta) = \theta^c \times (1-\theta)^l$

The maximum-likelihood hypothesis is given by the value of θ that maximizes this expression. This is equivalent to maximizing the log likelihood:

$$L(\mathbf{d}|h_\theta) = \log P(\mathbf{d}|h_\theta) = \sum_{j=1}^{N} P(d_j|h_\theta) = c\log\theta + l\log(1-\theta)$$

To find maximum-likelihood value of θ, differentiate L wrt θ, and set result to zero:

$$\frac{dL(\mathbf{d}|h_\theta)}{d\theta} = \frac{c}{\theta} - \frac{l}{1-\theta} = 0 \Rightarrow \theta = \frac{c}{c+l} = \frac{c}{N}$$

Thus, h_{ML} says proportion of cherries in bag = proportion observed so far.

Standard Method for ML Parameter Learning

1. Write down an expression for the likelihood of the data as a function of the parameter(s).
2. Write down the derivative of the log likelihood with respect to each parameter.
3. Find the parameter values such that the derivatives are zero.

Problem: When data set is small enough so that some events have not yet been observed, the maximum likelihood hypothesis assigns zero probability to those events.

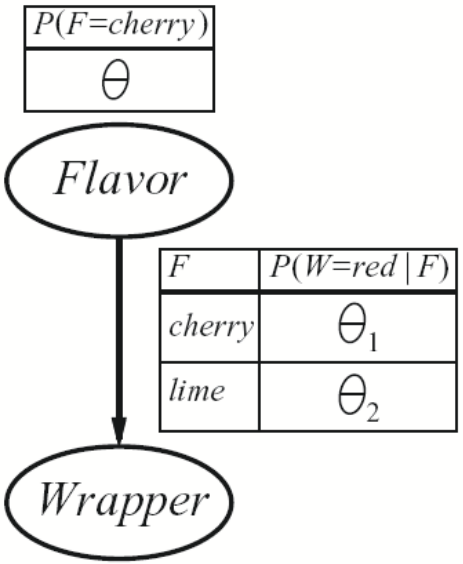
Possible solutions: initialize counts for each event to 1 instead of 0.

Another Example: Add Wrappers

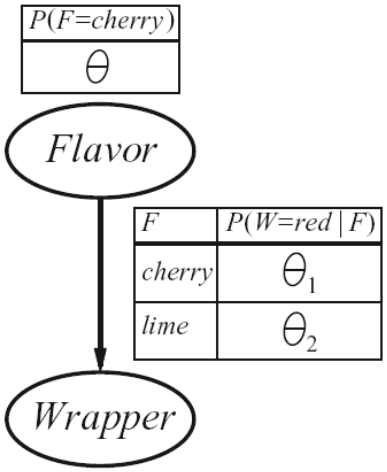
Red and green wrappers assigned probabilistically, depending on flavor.

Now have 3 parameters: θ, θ_1, θ_2.

Corresponding Bayesian network:



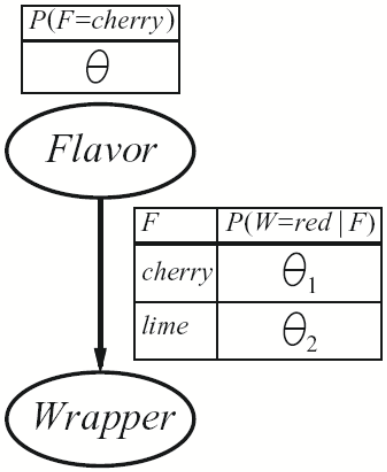
Another Example: Add Wrappers



Remember standard semantics of Bayesian Nets... (Note that here we're showing the parameters as given info, just to make it explicit; normally, the parameters are implicitly assumed as given info.)

$$P(Flavor = cherry, Wrapper = green | h_\theta, h_{\theta_1}, h_{\theta_2})$$

Another Example: Add Wrappers

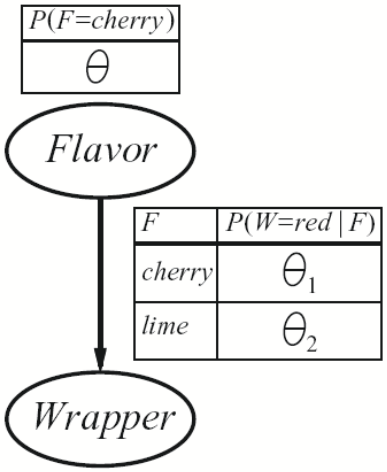


Remember standard semantics of Bayesian Nets... (Note that here we're showing the parameters as given info, just to make it explicit; normally, the parameters are implicitly assumed as given info.)

$$P(Flavor = cherry, Wrapper = green | h_\theta, h_{\theta_1}, h_{\theta_2})$$

$$= P(Flavor = cherry | h_\theta, h_{\theta_1}, h_{\theta_2})$$
$$\times P(Wrapper = green | Flavor = cherry, h_\theta, h_{\theta_1}, h_{\theta_2})$$

Another Example: Add Wrappers



Remember standard semantics of Bayesian Nets... (Note that here we're showing the parameters as given info, just to make it explicit; normally, the parameters are implicitly assumed as given info.)

$$P(Flavor = cherry, Wrapper = green | h_\theta, h_{\theta_1}, h_{\theta_2})$$

$$= P(Flavor = cherry | h_\theta, h_{\theta_1}, h_{\theta_2}) \times P(Wrapper = green | Flavor = cherry, h_\theta, h_{\theta_1}, h_{\theta_2})$$

$$= \theta \cdot (1 - \theta_1)$$

Another Example: Add Wrappers

Now, unwrap N candies, of which c are cherry and l are lines.

r_c of cherries have red wrappers;
g_c of cherries have green wrappers;
r_l of limes have red wrappers;
g_l of limes have green wrappers.

Likelihood of data:

$$P(\mathbf{d}|h_\theta, h_{\theta_1}, h_{\theta_2}) = \theta^c(1-\theta)^l \cdot \theta_1^{r_c}(1-\theta_1)^{g_c} \cdot \theta_2^{r_l}(1-\theta_2)^{g_l}$$

Taking logs gives us:

$$\begin{aligned} L = & \left[c\log\theta + l\log(1-\theta)\right] + \left[r_c\log\theta_1 + g_c\log(1-\theta_1)\right] \\ & + \left[r_l\log\theta_2 + g_l\log(1-\theta_2)\right] \end{aligned}$$

Another Example: Add Wrappers

$$L = [c \log \theta + l \log(1-\theta)] + [r_c \log \theta_1 + g_c \log(1-\theta_1)] + [r_l \log \theta_2 + g_l \log(1-\theta_2)]$$

Take derivatives wrt each parameter and set to 0 gives us:

$$\frac{\partial L}{\partial \theta} = \frac{c}{\theta} - \frac{l}{1-\theta} = 0 \Rightarrow \theta = \frac{c}{c+l}$$

$$\frac{\partial L}{\partial \theta_1} = \frac{r_c}{\theta_1} - \frac{g_c}{1-\theta_1} = 0 \Rightarrow \theta_1 = \frac{r_c}{r_c+g_c}$$

$$\frac{\partial L}{\partial \theta_2} = \frac{r_l}{\theta_2} - \frac{g_l}{1-\theta_2} = 0 \Rightarrow \theta_2 = \frac{r_l}{r_l+g_l}$$

Important point 1: with complete data, ML parameter learning for a Bayesian network decomposes into separate learning problems, one for each parameter.

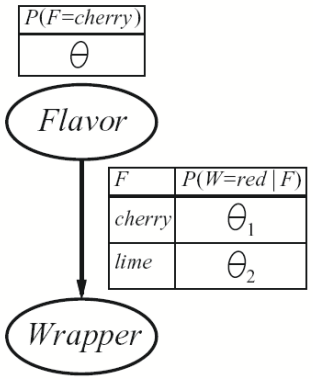
Important point 2: parameter values for a variable, given its parents, are the observed freq. of the variable values for each setting of the parent values.

Naive Bayes Models

Naive Bayes Model = Most common Bayesian network model

Representation: "Class" variable (C) is the root, and "attribute" variables (X_i) are the leaves.

Example of Naive Bayes Model with one attribute:



"Naive" $\Rightarrow$ assumes attributes are conditionally independent, given the class.

Objective: after learning, predict "Class" of new examples

$$\mathbf{P}(C|x_1, ...x_n) = \alpha \mathbf{P}(C) \prod_i \mathbf{P}(x_i|C)$$

Naive Bayes Models (con't)

Nice characteristics of Naive Bayes learning:

- Works surprisingly well in wide range of applications
- Scales well to very large problems (n Boolean attributes $\Rightarrow 2n + 1$ parameters)
- No search is required to find h_{ML}
- No difficulty with noisy data
- Can give probabilistic predictions when appropriate

Naive Bayes Classifier Example

We want to build a classifier that can classify days according to whether someone will play tennis. How do we start?

Naive Bayes Classifier Example

Day	Outlook	Temp	Humidty	Wind	Play?
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Naive Bayes Classifier Example

Now, we have a new instance we want to classify:
(Outlook = Sunny, Temp = Cool, Humidity = High, Wind = Strong)

Need to predict 'Yes' or 'No'.

What now?

Naive Bayes Classifier Example

Now, we have a new instance we want to classify:
(Outlook = Sunny, Temp = Cool, Humidity = High, Wind = Strong)

Need to predict 'Yes' or 'No'.

What now?

Let v be either 'Yes' or 'No'.

Then,

$$v = \text{argmax}_{v_j \in [Yes,No]} P(v_j) \prod_i P(x_i|v_j)$$

$$= \text{argmax}_{v_j \in [Yes,No]} P(v_j) \times P(\text{Outlook=Sunny}|v_j) \times P(\text{Temp=Cool}|v_j)$$

$$\times P(\text{Humidity=High}|v_j) \times P(\text{Wind=Strong}|v_j)$$

Naive Bayes Classifier Example

$P(\text{Play?=Yes}) =$

$P(\text{Play?=No}) =$

$P(\text{Outlook=Sunny}|\text{Play?=Yes}) =$

$P(\text{Outlook=Sunny}|\text{Play?=No}) =$

$P(\text{Temp=Cool}|\text{Play?=Yes}) =$

$P(\text{Temp=Cool}|\text{Play?=No}) =$

$P(\text{Humidity=High}|\text{Play?=Yes}) =$

$P(\text{Humidity=High}|\text{Play?=No}) =$

$P(\text{Wind=Strong}|\text{Play?=Yes}) =$

$P(\text{Wind=Strong}|\text{Play?=No}) =$

Naive Bayes Classifier Example

$P(\text{Play?=Yes}) = 9/14 = 0.64$

$P(\text{Play?=No}) = 5/14 = 0.36$

$P(\text{Outlook=Sunny}|\text{Play?=Yes}) = 2/9 = 0.22$

$P(\text{Outlook=Sunny}|\text{Play?=No}) = 3/5 = 0.60$

$P(\text{Temp=Cool}|\text{Play?=Yes}) = 3/9 = 0.33$

$P(\text{Temp=Cool}|\text{Play?=No}) = 1/5 = 0.20$

$P(\text{Humidity=High}|\text{Play?=Yes}) = 3/9 = 0.33$

$P(\text{Humidity=High}|\text{Play?=No}) = 4/5 = 0.80$

$P(\text{Wind=Strong}|\text{Play?=Yes}) = 3/9 = 0.33$

$P(\text{Wind=Strong}|\text{Play?=No}) = 3/5 = 0.60$

Naive Bayes Classifier Example

And, what is decision? Yes or No?

Naive Bayes Classifier Example

And, what is decision? Yes or No?

$$P(\text{Yes})P(\text{Sunny}|\text{Yes})P(\text{Cool}|\text{Yes})P(\text{High}|\text{Yes})P(\text{Strong}|\text{Yes})$$

$$= 0.64 \times 0.22 \times 0.33 \times 0.33 \times 0.33 = 0.0051$$

$$P(\text{No})P(\text{Sunny}|\text{No})P(\text{Cool}|\text{No})P(\text{High}|\text{No})P(\text{Strong}|\text{No})$$

$$= 0.36 \times 0.60 \times 0.20 \times 0.80 \times 0.60 = 0.0207$$

Conditional probability that value is "No":

$$\frac{0.0207}{0.0207 + 0.0051} = 0.80$$

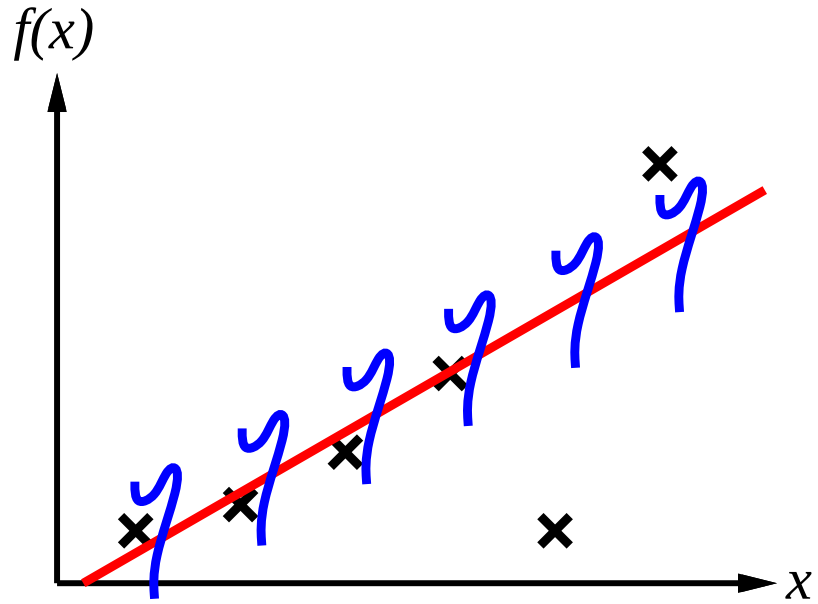
No tennis today.

ML Parameter Learning: Continuous Models

How to learn continuous models from data? Very similar to discrete case.

Data: pairs $(x_1, y_1), \ldots, (x_N, y_N)$

Hypotheses: straight lines $y = ax + b$ with Gaussian noise
Want to choose parameters $\theta = (a, b)$ to maximize likelihood of data (this is linear regression)



Recall: Method for ML Parm Learning

1. Write down an expression for the likelihood of the data as a function of the parameter(s).
2. Write down the derivative of the log likelihood with respect to each parameter.
3. Find the parameter values such that the derivitives are zero.

ML Parameter Learning: Cont. Models (con't.)

Data assumed i.i.d. (independently and identically distributed)

$\Rightarrow$ likelihood $P(\mathbf{d}|h_i) = \prod_j P(d_j|h_i)$

Maximizing likelihood $P(\mathbf{d}|h_i)$ $\Leftrightarrow$ maximizing log likelihood

$$L = \log P(\mathbf{d}|h_i) = \log \prod_j P(d_j|h_i) = \sum_j \log P(d_j|h_i)$$

For a continuous hypothesis space, set $\partial L/\partial\theta = 0$ and solve for θ

For Gaussian noise, $P(d_j|h_i) = \alpha \exp\left(-(y_j - (ax_j + b))^2/2\sigma^2\right)$, so

$$L = \sum_j \log P(d_j|h_i) = -\alpha' \sum_j (y_j - (ax_j + b))^2$$

so maximizing L = minimizing sum of squared errors

Note: This is just standard linear regression! That is, linear regression is the same thing as maximum-likelihood (ML) learning (as long as data are generated with Gaussian noise of fixed variance).

ML Parameter Learning: Cont. Models (con't.)

To find the maximum, set derivatives to zero:

$$\frac{\partial L}{\partial a} = -\alpha' \Sigma_j \, 2(y_j - (ax_j + b)) \cdot (-x_j) = 0$$
$$\frac{\partial L}{\partial b} = -\alpha' \Sigma_j \, 2(y_j - (ax_j + b)) \cdot (-1) = 0$$

Solve for parameters a and b. Solutions are:

$$a = \frac{\Sigma_j \, x_j \Sigma_j \, y_j - N \Sigma_j \, x_j y_j}{\left(\Sigma_j \, x_j\right)^2 - N \Sigma_j \, x_j^2} \; ; \quad b = \left(\Sigma_j \, y_j - a \, \Sigma_j \, x_j\right) / N$$

ML learning with Continuous Models

Let's assume we have m data points (x_j, y_j), where y_j's generated from x_j's according to the following linear Gaussian model:

$$P(y|x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-(\theta_1 x+\theta_2))^2}{2\sigma^2}}$$

Find the values of θ_1, θ_2, and σ that maximize the conditional log likelihood of the data.

ML learning with Continuous Models

Let's assume we have m data points (x_j, y_j), where y_j's generated from x_j's according to the following linear Gaussian model:

$$P(y|x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-(\theta_1 x+\theta_2))^2}{2\sigma^2}}$$

Find the values of θ_1, θ_2, and σ that maximize the conditional log likelihood of the data.

Likelihood of this data set is:

$$\prod_{j=1}^{m} P(y_j|x_j)$$

Then, compute log likelihood, take derivative, set equal to 0, and solve for the 3 parameters.

Learning Bayes Net structures

What if structure of Bayes net is not known?

Techniques for learning are not well-established.

General idea: search for good model, then measure its quality.

Searching for a good model

Option 1: Start with no links, and add parents for each node, fitting the parameters, and then measuring the accuracy of the result.

Option 2: Guess a structure, then use hill-climbing, simulated annealing, etc., to improve, re-tuning the parameters after each step.

Learning Bayes Net structures (con't.)

How to measure quality of structure?

Option 1: Test whether conditional independence assertions implicit in the structure are actually satisfied in the data.

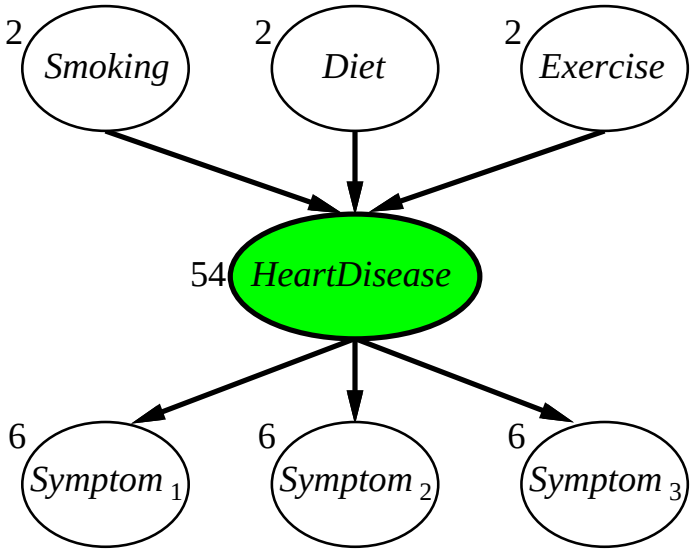
Option 2: Measure the degree to which model explains the data (probabilistically).

Problem: fully connected network will have high correlation to data. So, need to penalize for complexity. Usually, use MCMC for sampling over structures.

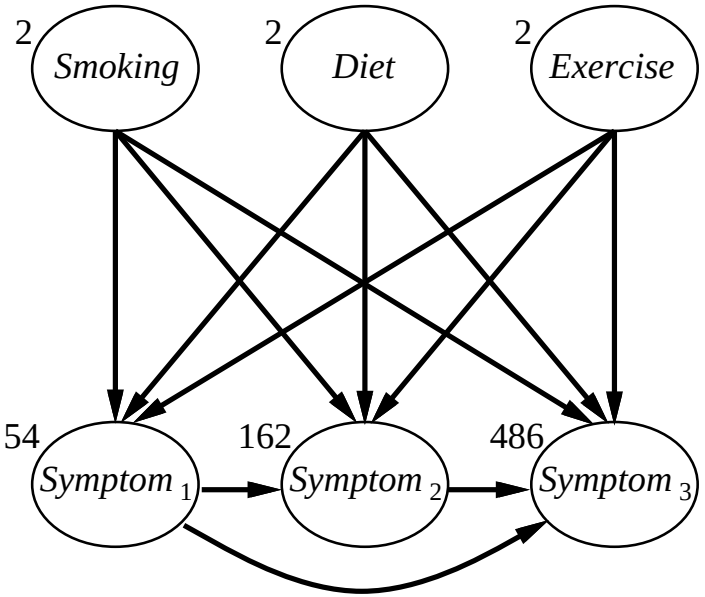
Learning with Hidden Variables

Hidden (or latent) variables: not observable in data

Hidden variables can dramatically reduce number of parameters needed to specify a Bayesian network $\Rightarrow$ dramatically reduce amount of data needed to learn parameters



(a)



(b)

Expectation-Maximization (EM) Algorithm

Solves problem in general way

Applicable to huge range of learning problems

2-step process in each iteration (i.e., repeat until convergence):

- E-step (i.e., Expectation step): compute expected values of hidden variables (below, it's the summation)
- M-step (i.e., Maximization step): find new values of parameters that maximize log likelihood of data, given expected values of hidden variables

General form of EM algorithm:

$\mathbf{x}$: all observed values in examples
$\mathbf{Z}$: all hidden variables for all examples
θ: all parameters for probability model

$$\theta^{(i+1)} = \text{argmax}_\theta \sum_{\mathbf{Z}} P(\mathbf{Z} = \mathbf{z}|\mathbf{x}, \theta^{(i)}) L(\mathbf{x}, \mathbf{Z} = \mathbf{z}|\theta)$$

Using EM Algorithm

Starting from the general form, it is possible to derive an EM algorithm for a specific application once the appropriate hidden variables have been identified.

Examples:

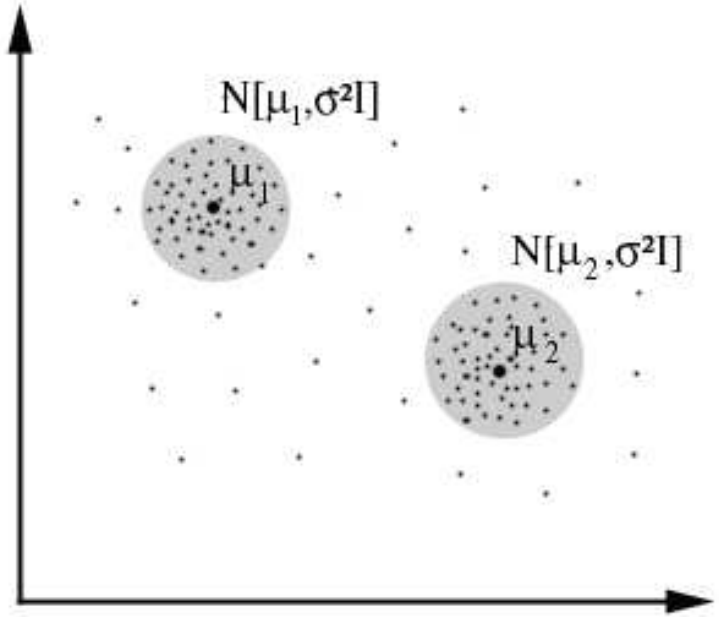
- ♢ Learning mixtures of Gaussians (unsupervised clustering)
- ♢ Learning Bayesian networks with hidden variables
- ♢ Learning hidden Markov models

EM Ex. 1: Unsupervised Clustering

Unsupervised clustering: discerning multiple categories in a collection of objects

Mixtures of Gaussians: combination of Gaussian "component" distributions

Example of Gaussian mixture model with 2 components:



Unsupervised Clustering (con't.)

Data are generated from mixture distribution P.

Distribution P has k components, each of which is itself a distribution

Let C = component, with values $1, ..., k$.

Let $\mathbf{x}$ = values of attributes of data point.

Then, mixture distribution is:

$$P(\mathbf{x}) = \sum_{i=1}^{k} P(C = i) P(\mathbf{x} | C = i)$$

Parameters of a mixture of Gaussians:

$w_i = P(C = i)$: the weight of each component
μ_i: mean of each component
Σ_i: the covariance of each component

Unsupervised clustering objective: learn mixture model from raw data.

Unsupervised Clustering Challenge

If we knew which component generated each data point, then it is easy to recover the component Gaussians – just select all the data points from a given component and apply ML parameter learning (like eqn. (20.4)).

Or, if we know the parameters of each component, we could probabilistically assign each data point to a component.

Problem:

Unsupervised Clustering Challenge

If we knew which component generated each data point, then it is easy to recover the component Gaussians – just select all the data points from a given component and apply ML parameter learning (like eqn. (20.4)).

Or, if we know the parameters of each component, we could probabilistically assign each data point to a component.

Problem: We don't know either.

Unsupervised Clustering (con't.)

Approach:

- Pretend we know the parameters of the model, and infer the probability that each data point belongs to each component
- Then, retrofit the components to the data, where each component is fitted to entire data set with each point weighted by the probability that it belongs to that component.

Iterate until convergence.

What is "hidden" in unsupervised clustering?

Unsupervised Clustering (con't.)

Approach:

- Pretend we know the parameters of the model, and infer the probability that each data point belongs to each component
- Then, retrofit the components to the data, where each component is fitted to entire data set with each point weighted by the probability that it belongs to that component.

Iterate until convergence.

What is "hidden" in unsupervised clustering?

We don't know which component each data set belongs to.

Unsupervised Clustering (con't.)

Two-step algorithm:

1. E-step: Compute $p_{ij} = P(C = i|\mathbf{x}_j)$ (i.e., probability that $\mathbf{x}_j$ was generated by component i)

   $$p_{ij} = \alpha P(\mathbf{x}_j|C = i)P(C = i)$$

2. M-step: Compute new mean, covariance, and component weights:

   $$\mu_i \leftarrow \sum_j p_{ij}\mathbf{x}_j/p_i$$

   $$\Sigma_i \leftarrow \sum_j p_{ij}\mathbf{x}_j\mathbf{x}_j^\top/p_i$$

   $$w_i \leftarrow p_i$$

Iterate until converge to a solution.

Some potential problems

♢ One Gaussian component could shrink to cover just a single data point; then, variance goes to 0 and its likelihood goes to infinity!

♢ Two components can merge, acquiring identical means and variances, and sharing data points.

Possible solutions:

♢ Place priors on model parameters and apply the MAP version of EM.

♢ Restart a component with new random parameters if it gets too small or too close to another component.

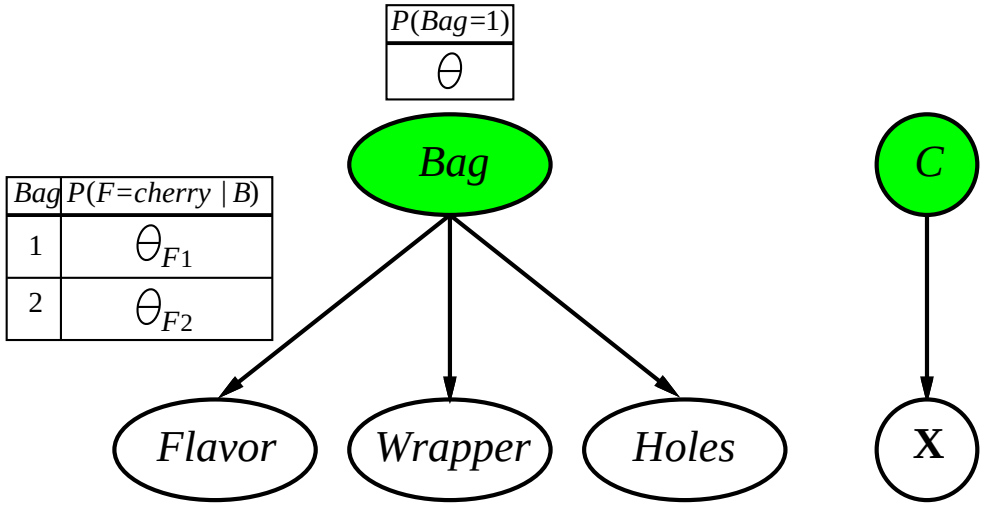
♢ Initialize the parameters with reasonable values.

EM Ex. 2: Bayesian NW with Hidden Vars

Two bags of candies mixed together.

Three features of candy: Flavor, Wrapper, Hole.

Distribution of candies in each bag described by Naive Bayes model (i.e., features are independent, given the bag, but CPT depends on bag)



Learning Bayesian NW with HV, con't.

Parameters:

θ: prior probability that candy comes from Bag 1

θ_{F1}, θ_{F2}: probabilities that flavor is cherry, given it comes from Bag 1 and Bag 2, respectively

θ_{W1}, θ_{W2}: probabilities that wrapper is red, given it comes from Bag 1 and Bag 2, respectively

θ_{H1}, θ_{H2}: probabilities that candy has hole, given it comes from Bag 1 and Bag 2, respectively

Hidden variable: the bag

Objective: Learn the descriptions of the two bags by observing candies from mixture

Learning Bayesian NW with HV, con't.

Let's step through iteration of EM.

Data: 1000 samples from model whose true parameters are:

$$\theta = 0.5$$
$$\theta_{F1} = \theta_{W1} = \theta_{H1} = 0.8$$
$$\theta_{F2} = \theta_{W2} = \theta_{H2} = 0.3$$

Data counts:

	W=red		W=green	
	H=1	H=0	H=1	H=0
F = cherry	273	93	104	90
F = lime	79	100	94	167

Learning Bayesian NW with HV, con't.

First, initialize parameters:

$$\theta^{(0)} = 0.6$$
$$\theta^{(0)}_{F1} = \theta^{(0)}_{W1} = \theta^{(0)}_{H1} = 0.6$$
$$\theta^{(0)}_{F2} = \theta^{(0)}_{W2} = \theta^{(0)}_{H2} = 0.4$$

Now, work on θ.

Because the bag is a hidden variable, we estimate this from expected counts: $\hat{N}(Bag = 1) =$ sum, over all candies, of probability that candy came from bag 1:

$$\theta^{(1)} = \hat{N}(Bag = 1)/N$$

$$= \sum_{j=1}^{N} P(B = 1|f_j, w_j, h_j)/N$$

$$\theta^{(1)} = \frac{1}{N}\sum_{j=1}^{N} \frac{P(f_j|B = 1)P(w_j|B = 1)P(h_j|B = 1)P(B = 1)}{\sum_i P(f_j|B = i)P(w_j|B = i)P(h_j|B = i)P(B = i)}$$

Learning Bayesian NW with HV, con't.

Apply to the 273 red-wrapped cherry candies with holes:

$$\frac{273}{1000} \cdot \frac{\theta_{F1}^{(0)}\theta_{W1}^{(0)}\theta_{H1}^{(0)}\theta^{(0)}}{\theta_{F1}^{(0)}\theta_{W1}^{(0)}\theta_{H1}^{(0)}\theta^{(0)} + \theta_{F2}^{(0)}\theta_{W2}^{(0)}\theta_{H2}^{(0)}(1-\theta^{(0)})} \approx 0.22797$$

Applying to remaining 7 kinds of candy, we get $\theta^{(1)} = 0.6124$.

Now, look at θ_{F1}. Expected count of cherry candies from Bag 1 is:

$$\sum_{j:Flavor_j=cherry} P(Bag = 1 | Flavor_j = cherry, wrapper_j, holes_j)$$

Calculate these probabilities (using inference alg. for Bayes net):

$\theta^{(1)} = 0.6124$

$\theta_{F1}^{(1)} = 0.6684$	$\theta_{W1}^{(1)} = 0.6483$	$\theta_{H1}^{(1)} = 0.6558$
$\theta_{F2}^{(1)} = 0.3887$	$\theta_{W2}^{(1)} = 0.3817$	$\theta_{H2}^{(1)} = 0.3827$

Main Lesson from Bayesian NW Learning

Main points:

- Parameter updates for Bayesian network learning with hidden variables are directly available from the results of inference on each example (so, no extra computations specific to learning).
- Only *local* posteriori probabilities are needed for each parameter.

In general, for learning conditional probability parameters for each variable X_i, given its parents (i.e., $\theta_{ijk} \leftarrow P(X_i = x_{ij}, Pa_i = pa_{ik})$), the update is given by normalized expected counts:

$$\theta_{ijk} \leftarrow \hat{N}P(X_i = x_{ij}, Pa_i = pa_{ik})/\hat{N}(Pa_i = pa_{ik})$$

Expected counts are obtained by summing over the examples and computing the probabilities $P(X_i = x_{ij}, Pa_i = pa_{ik})$ using a Bayes net inference algorithm.

EM Ex. 3: Learning HMMs

In Hidden Markov Models, hidden variables are the $i \rightarrow j$ transitions.

Each data point: finite observation sequence

Objective: learn transition probabilities from sequences

Similar to learning Bayesian nets with hidden variables.

Complication: In Bayes nets, each parameter is distinct. In HMM, individual transition probabilities from state i to state j are repeated across time (i.e., $\theta_{ijt} = \theta_{ij}$ for all t)

Thus, to estimate transition probability from state i to state j, we calculate expected proportion of times that the system undergoes transition to state j when in state i:

$$\theta_{ij} \leftarrow \Sigma_t \hat{N}(X_{t+1} = j, X_{t=i}) / \Sigma_t \hat{N}(X_{t=i})$$

Learning HMMs (con't.)

Similar to learning Bayesian NWs, here we can compute expected counts by any HMM inference algorithm.

E.g., the forward-backward algorithm of smoothing (Fig. 15.4) can be used (modified easily to compute the required probabilities). This algorithm is also known as **Baum-Welch** algorithm.

Note: we're making use of **smoothing** instead of **filtering**, since we need to pay attention to subsequent evidence in estimating the probability that a particular transition occurred.

The forward-backward (Baum-Welch) algorithm is a particular case of the generalized EM. It computes maximum likelihood estimate of the parameters of the HMM given a sequence of outputs.

Summarizing: General EM Algorithm

Expectation Maximization algorithm:

2-step process:

- E-step (i.e., Expectation step): compute expected values of hidden variables (below, it's the summation)
- M-step (i.e., Maximization step): find new values of parameters that maximize log likelihood of data, given expected values of hidden variables

General form of EM algorithm:

$\mathbf{x}$: all observed values in examples
$\mathbf{Z}$: all hidden variables for all examples
θ: all parameters for probability model

$$\theta^{(i+1)} = \text{argmax}_\theta \sum_{\mathbf{Z}} P(\mathbf{Z} = \mathbf{z}|\mathbf{x}, \theta^{(i)}) L(\mathbf{x}, \mathbf{Z} = \mathbf{z}|\theta)$$

Summary

Full Bayesian learning gives best possible predictions but is intractable

MAP learning balances complexity with accuracy on training data

Maximum likelihood assumes uniform prior, OK for large data sets

ML for continuous spaces using gradient of log likelihood

Regression with Gaussian noise $\longrightarrow$ minimize sum-of-squared errors

When some variables are hidden, local maximum likelihood solutions can be found using Expectation Maximization algorithm.

Applications of EM: clustering using mixtures of Gaussians, learning Bayesian networks, learning hidden Markov models