Graphical Models

Bayesian Networks

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Objectives

Objective

Describe Bayesian Networks

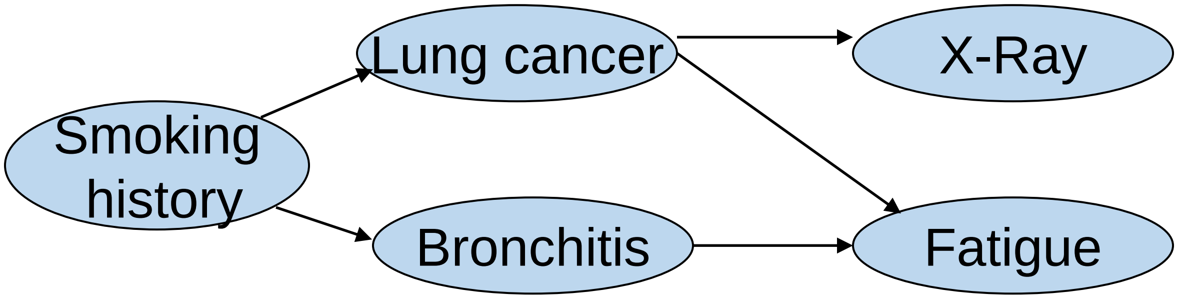
Objective

Illustrate key tasks in implementing Bayesian Networks

Why do we use graphical models?

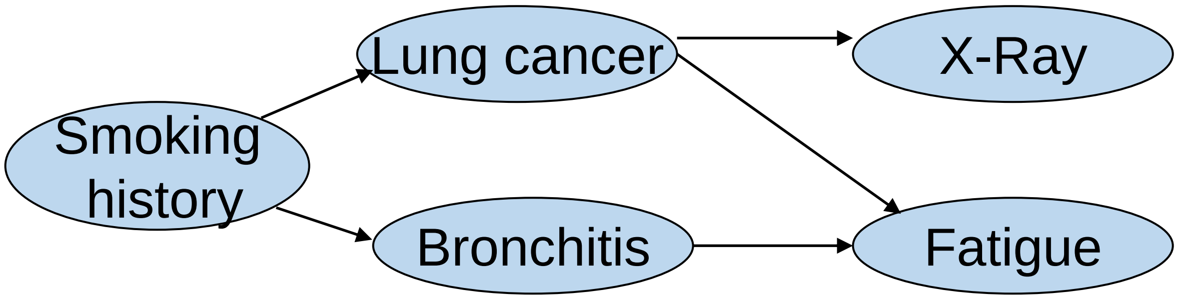
- **In machine learning, we are often concerned with joint distributions of many random variables.**

- **A graph may provide an intuitive way of representing or visualizing the relationships of the variables.**
  - Making it easier for domain experts to build a model



Graphical Models for Casual Relations

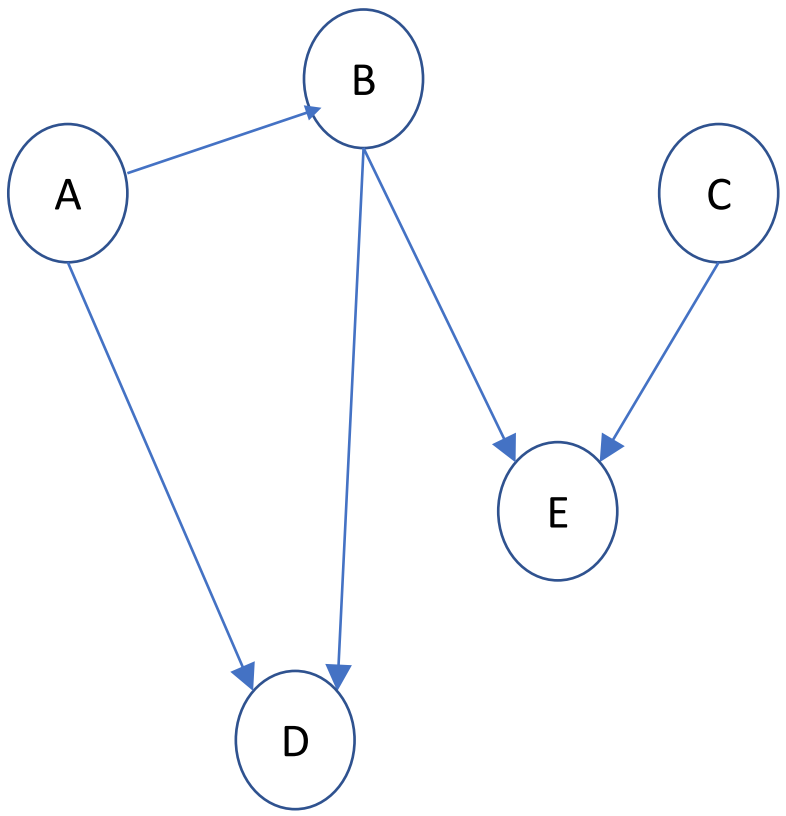
- **Graphical models arise naturally from, often causal, independency relations of physical events.**



- **Caveat: probabilistic relationship does not imply causality.**

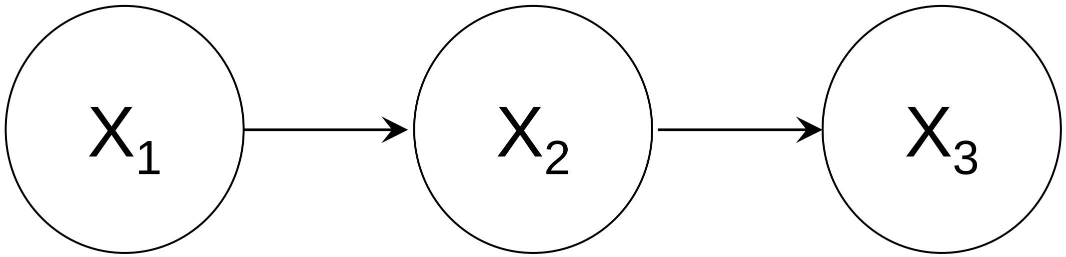
Bayesian Networks

- **A BN is directed acyclic graph (DAG), where**
  - Nodes (vertices) represent random variables.
  - Directed edges represent immediate dependence of nodes.
- **Other names: Belief networks, Bayes nets, etc.**



Conditional Independence

- **E.g., given the following graph, check the relationship between X_3 and X_1**



  - X_3 is dependent of X_2, and X_2 is dependent of X_1
  - Thus X_3 is dependent of X_1
  - But given X_2, X_3 is dependent of X_1

➔ Conditional Independence

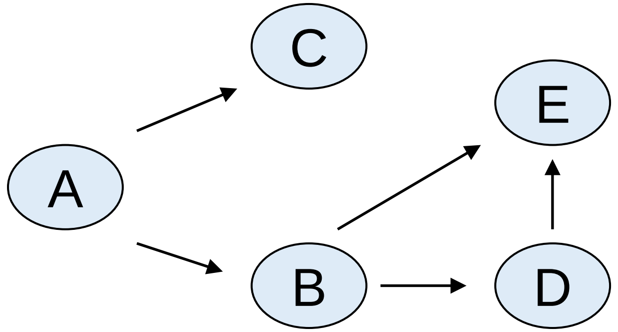
BN for General Conditional Dependency

- **A BN can be used to model given conditional dependencies**
  - For example, using the *chain rule of probability*, we have

$$P(A,B,C,D,E)=P(A)P(B|A)P(C|A,B)P(D|A,B,C)P(E|A,B,C,D)$$

- **If we know that, given A, C won't rely on B, and so forth, we may have**

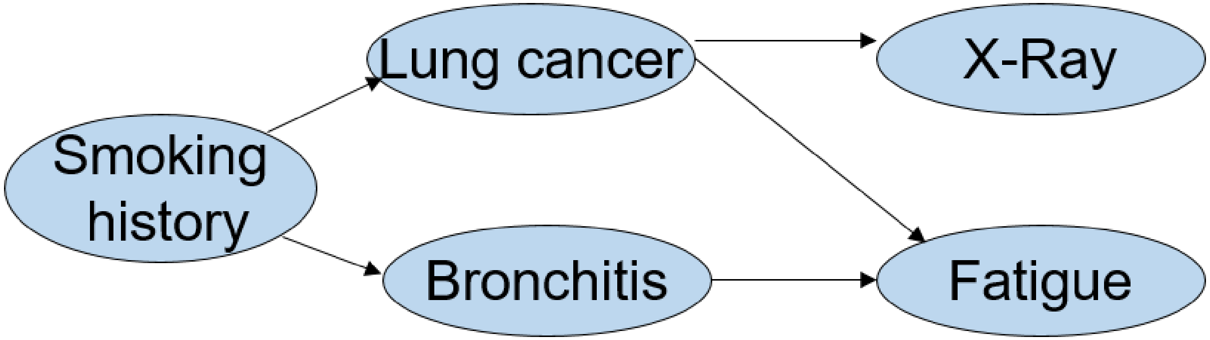
$$P(A,B,C,D,E)=P(A)P(B|A)P(C|A)P(D|B)P(E|B,D)$$



➢ We could represent joint distributions more compactly in BN → Efficient computation

Inference in Bayesian Networks

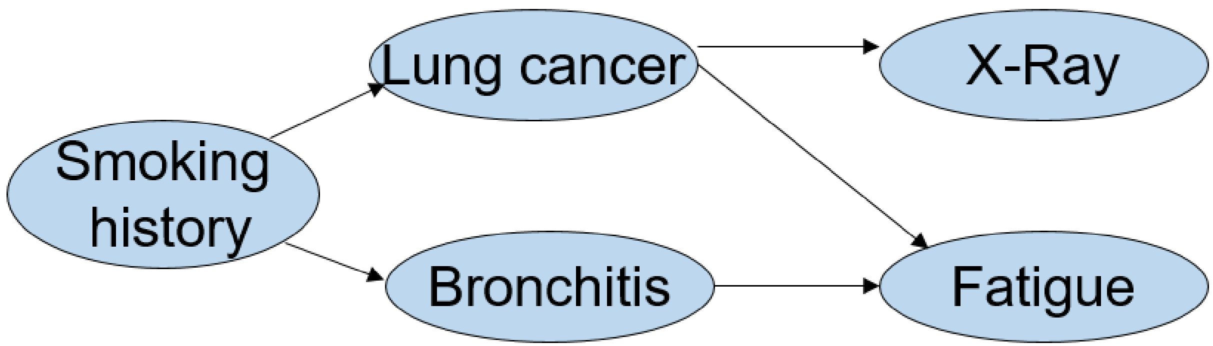
- **Given a model and some data ("evidence"), how to update our belief?**



- **What are the model parameters?**

Inference in Bayesian Networks (cont'd)

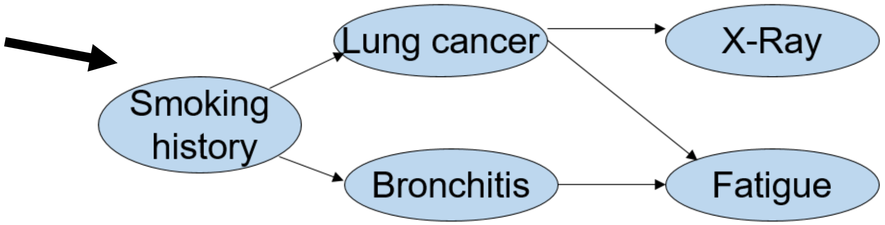
- **Given a model and some data ("evidence"), how to update our belief?**



- **E.g., for a patient with certain smoking history (non-smoker), whose X-ray result is positive, and who does not experience fatigue:**
  - What is probability of having lung cancer?

Inference in Bayesian Networks (cont'd)

- **In a simple BN like this, we can compute the exact probabilities.**



- **In general, for a tree-structured BN, we may use belief propagation for the inference problem.**
- **For general structures, sometimes it is possible to generalize the above method (e.g., the *junction tree algorithm*). More often, we must resort to approximation methods**
  - E.g. Variational methods, Sampling (Monte Carlo) methods.

Learning in Bayesian Networks

- **Learning parameters (probabilities) for a given BN (the graph is given).**
  - Estimate the (conditional) probabilities from past data.

- **Learning both the structure and the parameters for a BN**
  - A more challenging task beyond the scope of this discussion.

Learning the Probabilities

Basic ideas

- Use relative frequency for estimating probability.
- A prior distribution is typically assumed.
- The prior is then updated by the data into posterior.
- Using the MLE principle

The so-called “Expectation-Maximization (EM) Algorithm” is often used.

- Iteratively update our guess for the parameter and each step attempts to apply the MLE principle.

Graphical Models

Hidden Markov Formulation

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Objectives

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Introduce Hidden Markov Models

Objective

Illustrate HMM with intuitive examples

Hidden Markov Models

- **Hidden Markov Models (HMMs) are a type of dynamic Bayesian Network**
  - Modeling a process indexed by time
- **“Hidden”: the observations are due to some underlying (hidden) states not directly observable.**
- **“Markov”: the state transitions are governed by a Markov process.**

Discrete Markov Process

- **Consider a system which may be described at any time as being in one of a set of N distinct states, S_1, …, S_N.**
- **At time instances $t=1,2,3$, …, the system changes its state according to certain probability. The full description requires us to know $P(s^t=S_j \mid s^{t-1}=S_i, s^{t-2}=S_k, \ldots, s^1=S_m)$ for all $t, i, k, \ldots, m$, where s^t stands for the state of the system at time t.**
  - For a first-order Markov chain, we need to consider only

$$P(s^t=S_j \mid s^{t-1}=S_i)$$

  - Further assume *P*s are "stationary":

$$a_{ij} = P(s^t=S_j \mid s^{t-1}=S_i),\ 1 \le i,j \le N, \text{ for any } t.$$

A Simple Example

- **Assume one of the three states for each day:**

  S_1-rainy, S_2-cloudy, S_3-sunny

- **Assume the transition probability matrix**

$$A = \{a_{ij}\} = \begin{bmatrix} 0.5 & 0.2 & 0.3 \\ 0.3 & 0.3 & 0.4 \\ 0.1 & 0.2 & 0.7 \end{bmatrix}$$

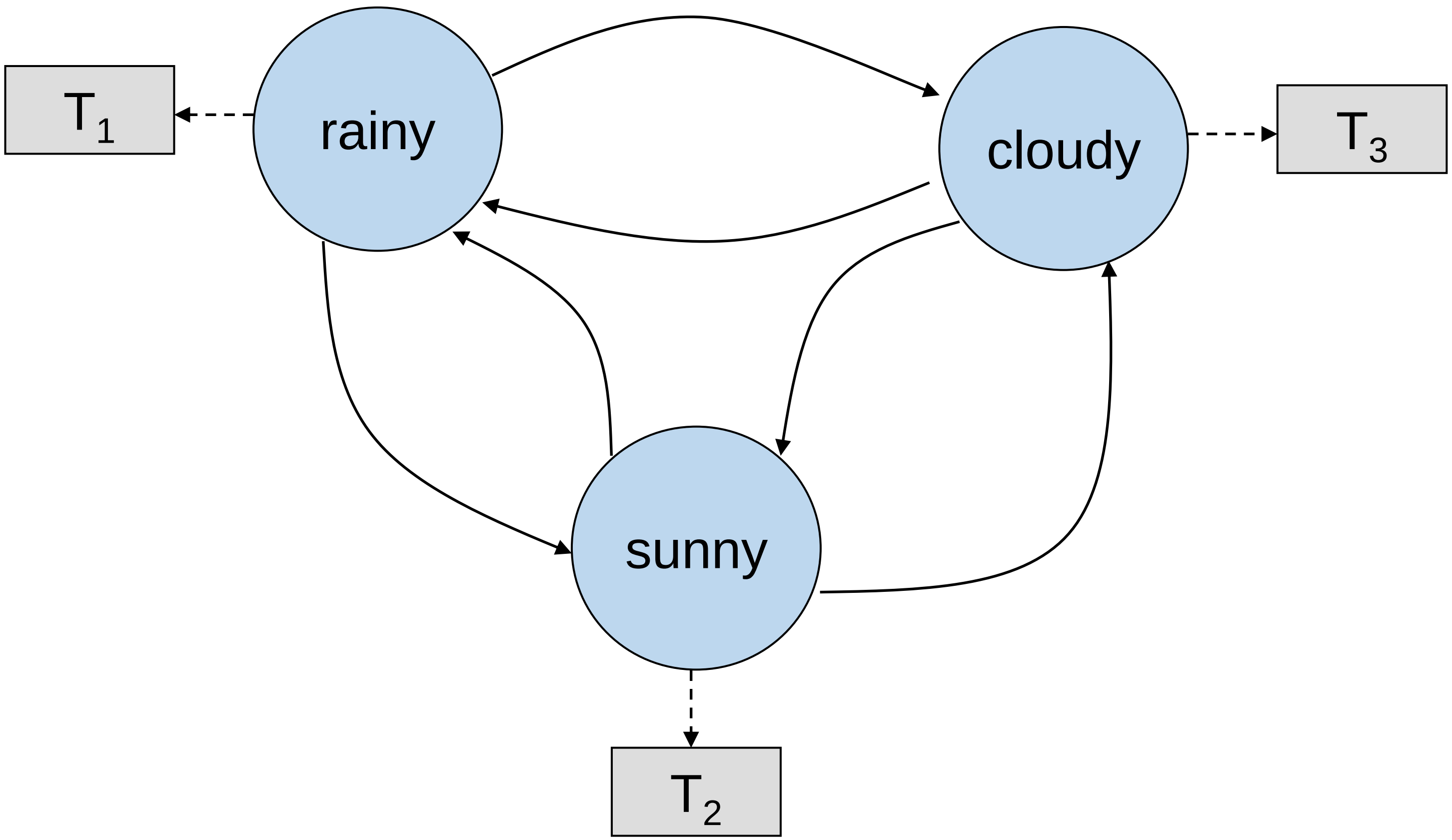
- **Many questions we may ask, based on this model.**
  - E.g., Given today is cloudy, what is the probability it remains to be cloudy for next 5 days?

Extending to “Hidden” States

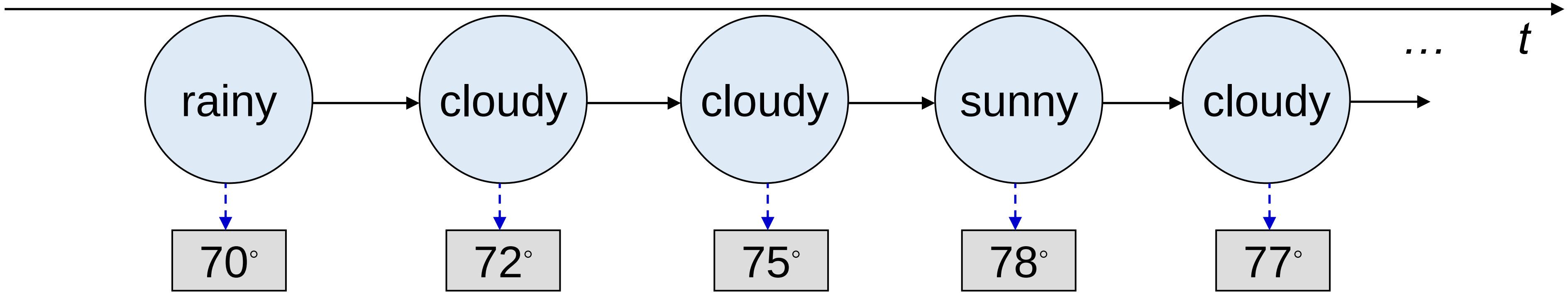
- **The previous example is an “observable” Markov model: the output of the system/process is the states of interest.**

- **Now assume that we can only measure the (average) temperature of a day**
  - Further assume this measurement is useful for predicting the weather states (rainy, cloudy, sunny).
  - We can view the temperature values as being produced by the *hidden states* of interest, i.e., the weather.

A Simple HMM



A Specific Process from the Model



Specifying an HMM

- **Θ: the set of hidden states.**

- **The state transition probabilities** $a_{ij} = P(s^t = S_j \mid s^{t-1} = S_i), 1 \le i,j \le N$
  - Let $A = \{a_{ij}\}$ be the transition probability matrix

- **Ω: the set of outputs (observations).**

Specifying an HMM (cont'd)

- **The observation probabilities: $P(o^t|s^t)$, where o^t stands for the observation at time t, given the state s^t. This is also called the emission probability.**
  - For discrete observation space, we can define $B=\{b_{jk}\}=P(o^t=\mathrm{v}_k \text{ at } t|s^t=S_j)$ as the emission probability matrix, where v_k is the k^{th} symbol in Ω

- **The initial state distribution $\pi = \{\pi_i\}$, $\pi_i=P(s^1=S_i)$**
  - Sometimes we are given an initial state, i.e., $P(s^1=S_i)=1$ for certain i.

Basic Problems in HMM

For a given HMM $\Lambda=\{\Theta,\Omega,A,B,\pi\}$

- Problem 1: Given an observation (sequence) $\boldsymbol{O}=\{o^1,o^2, \ldots ,o^k\}$, what is the most likely state sequence $\boldsymbol{S}=\{s^1,s^2, \ldots ,s^k\}$ that has produced $\boldsymbol{O}$?

- Problem 2: How likely is an observation $\boldsymbol{O}$ (i.e., what is $P(\boldsymbol{O})$) ?

- Problem 3: How to estimate the model parameters (A,B,π)?

Graphical Models

Hidden Markov Models: Learning & Inference

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Objective

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Implement HMM learning & inference algorithms

Basic Problems in HMM

For a given HMM $\Lambda=\{\Theta,\Omega,A,B,\pi\}$

- Problem 1: Given an observation (sequence) $\boldsymbol{O}=\{o^1,o^2, \ldots ,o^k\}$, what is the most likely state sequence $\boldsymbol{S}=\{s^1,s^2, \ldots ,s^k\}$ that has produced $\boldsymbol{O}$?

- Problem 2: How likely is an observation $\boldsymbol{O}$ (i.e., what is $P(\boldsymbol{O})$) ?

- Problem 3: How to estimate the model parameters (A,B,π)?

Problem 1: State Estimation

- Given an observation (sequence) $O=\{o^1,o^2, \ldots ,o^k\}$, what is the most likely state sequence $S=\{s^1,s^2, \ldots ,s^k\}$ that has produced O?

- Formally, we need to solve

$$\underset{\boldsymbol{S}}{\operatorname{argmax}} P(\boldsymbol{S}|\boldsymbol{O})$$

- Or, equivalently,

$$\underset{\boldsymbol{S}}{\operatorname{argmax}} \frac{P(\boldsymbol{S},\boldsymbol{O})}{P(\boldsymbol{O})} = \underset{\boldsymbol{S}}{\operatorname{argmax}} P(\boldsymbol{S},\boldsymbol{O})$$

Problem 1: State Estimation (cont'd)

- For a given HMM, we may simplify *P*(*S*,*O*) as

$$P(\boldsymbol{S},\boldsymbol{O}) = P(\boldsymbol{O}|\boldsymbol{S})P(\boldsymbol{S})$$

$$= P(o^1 \ldots o^k|s^1 \ldots s^k)\prod_{j=1}^{k} P(s^j|s^1 \ldots s^{j-1})$$

$$\simeq P(o^1 \ldots o^k|s^1 \ldots s^k)\prod_{j=1}^{k} P(s^j|s^{j-1})$$

$$= \prod_{i=1}^{k} P(o^i|o^1 \ldots o^{i-1}, s^1 \ldots s^i)\prod_{j=1}^{k} P(s^j|s^{j-1})$$

$$\simeq \prod_{i=1}^{k} P(o^i|s^i)\prod_{j=1}^{k} P(s^j|s^{j-1}) = \prod_{i=1}^{k} P(o^i|s^i)\, P(s^i|s^{i-1})$$

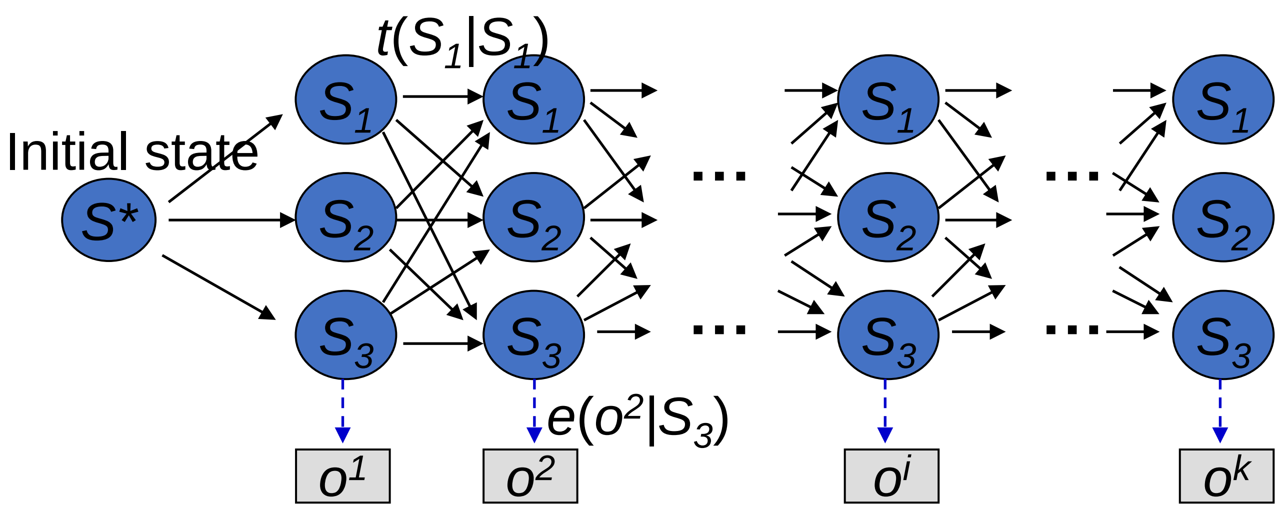
The "Weather" Example

Let's expand the state space as a trellis, for the earlier example:

S_1-rain, S_2-cloudy, S_3-sunny

-- $t(.|.)$ is the transition probability and $e(.|.)$ the emission probability.

➔ To identify a path for which the product of t's and the e's is maximized.



Viterbi Algorithm for Problem 1

A dynamic programming solution

– For each state in the trellis, we record:

1. $\delta_{s_i}(t)$ is the probability of taking the maximal path up to time *t-1* ending at state S_i at time *t* and while generating $o^1 \ldots o^t$

2. $\psi_{s_i}(t)$ is the state sequence that resulted in the maximal probability up to state S_i at time *t*.

Viterbi Algorithm (cont'd)

- **Initialization** $$\delta_{S_i}(1) = t(S_i|s^*)e(o^1|S_i), \quad \forall S_i \in \Theta$$

- **Induction:**
  for 2≤*t*≤*k*, do
  $$\delta_{S_i}(t) = \max_{S_j} t(S_i|S_j)e(o^t|S_i)\delta_{S_j}(t-1)$$
  $$\psi_{S_i}(t) = \operatorname*{argmax}_{S_j} t(S_i|S_j)e(o^t|S_i)\delta_{S_j}(t-1)$$

- **Termination:**
  - The probability of the best state sequence: $\max_{S_j} \delta_{S_j}(k)$
  - The best last state: $\hat{s}^k = \operatorname*{argmax}_{S_j} \delta_{S_j}(k)$
  - Back trace to get other states:
  $$\hat{s}^t = \psi_{\hat{s}^{t+1}}(t), \text{ for } t = k-1, \ldots, 1.$$

Problem 2: Evaluate *P*(*O*)

- To evaluate *P*(*O*), we can do $P(O) = \sum_{S} P(S, O)$

- From the trellis, a solution can be found by summing the probabilities of all paths generating the given observation sequence.

- A dynamic programming solution: <u>the forward algorithm</u> or the backward algorithm.

The Forward Algorithm

- **Define the forward probability $\alpha_{S_i}(t)$, which is the probability for all paths up to time *t-1* ending at state S_i at time *t* and generating $o^1 \ldots o^t$.**

1. Initialization: $\alpha_{S_i}(1) = t(S_i|s^*)e(o^1|S_i), \quad \forall S_i \in \Theta$

2. Induction:
   for $2 \le t \le k$, do $$\alpha_{S_i}(t) = \sum_{S_j} t(S_i|S_j)e(o^t|S_i)\alpha_{S_j}(t-1)$$

3. Termination: $$P(\boldsymbol{O}) = \sum_{S_j} \alpha_{S_j}(k)$$

Problem 3: Parameter Learning

Case 1: we have a set of labeled data – sequences in which we have the <state, observation> information

– Use relative frequency for estimating the probabilities

→ the MLE solution

$$t(S_i|S_j) = \frac{\text{number of } (s^t = S_i, s^{t-1} = S_j)}{\text{number of } S_j} \qquad e(o_r|S_j) = \frac{\text{number of } (o^t = o_r, s^t = S_j)}{\text{number of } S_j}$$

Case 2: we have only the observation sequence

– The Forward-Backward Algorithm (a.k.a. Baum-Welch Algorithm): An EM approach.