CS 1675: Intro to Machine Learning

Probabilistic Graphical Models

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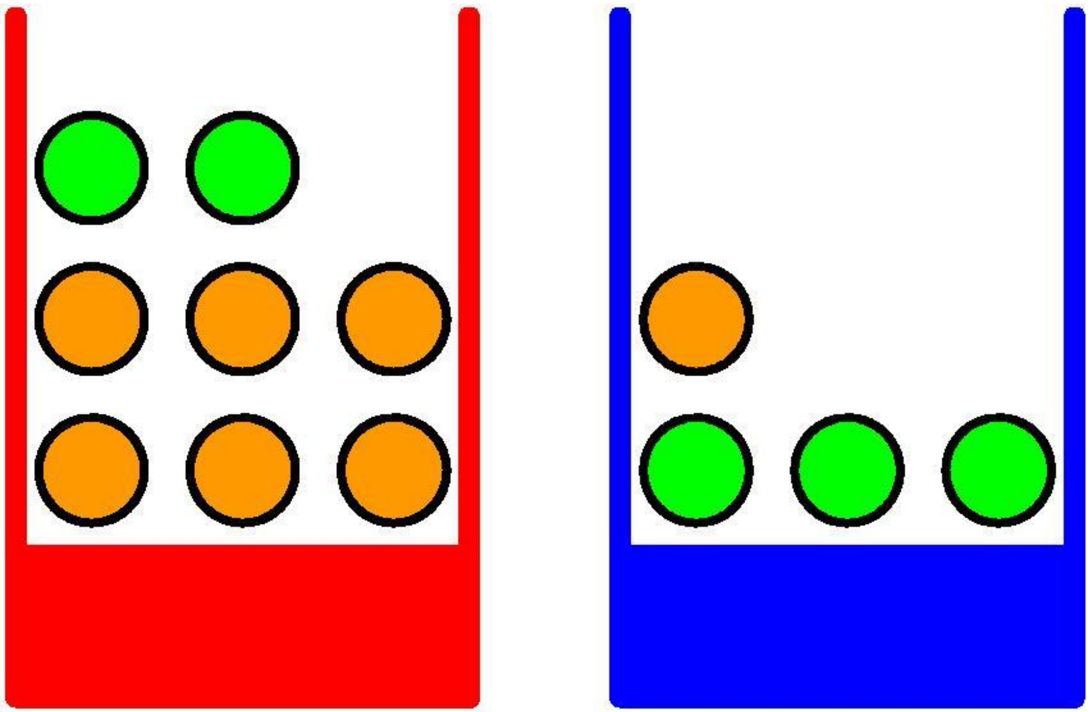
Plan for This Lecture

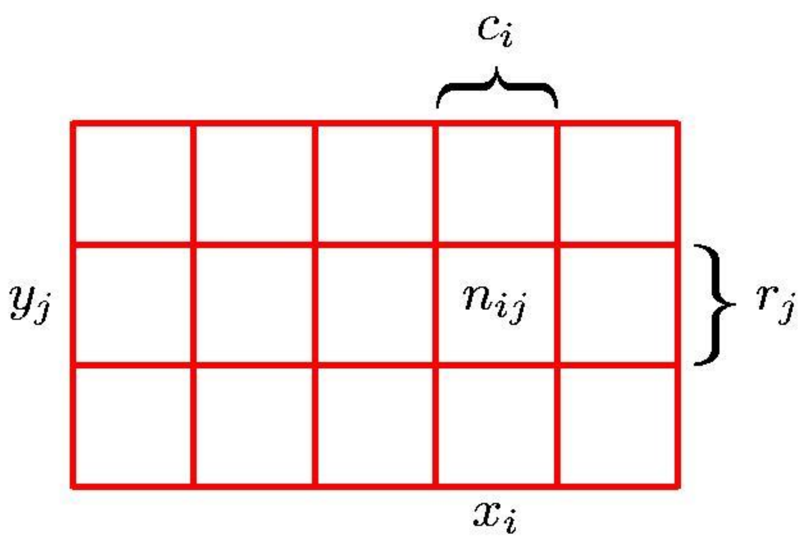
- Motivation for probabilistic graphical models
- Directed models: Bayesian networks
- Undirected models: Markov random fields (briefly)
- Directed models for sequence classification: Hidden Markov models

Probabilities: Example Use

Apples and Oranges



Marginal, Joint, Conditional



Marginal Probability

$$p(X = x_i) = \frac{c_i}{N}.$$

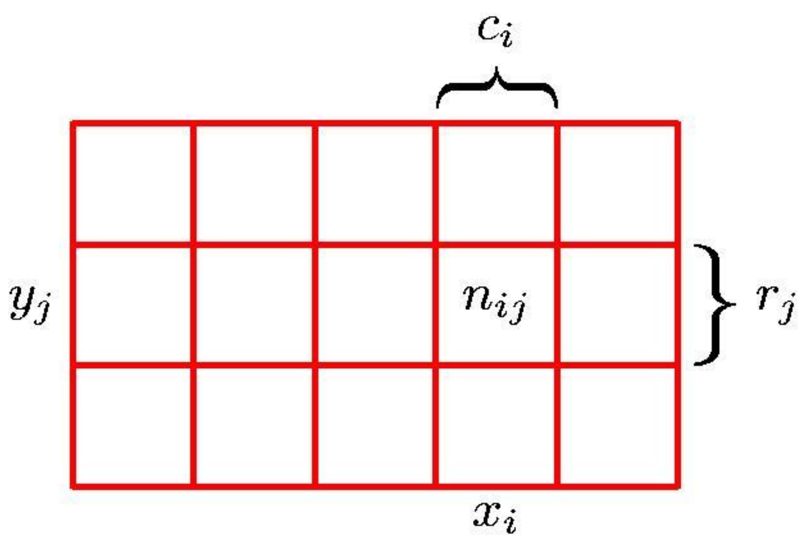
Joint Probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

Conditional Probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

Sum and Product Rules



Sum Rule

$$p(X = x_i) = \frac{c_i}{N} = \frac{1}{N}\sum_{j=1}^{L} n_{ij}$$

$$= \sum_{j=1}^{L} p(X = x_i, Y = y_j)$$

Product Rule

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$$

$$= p(Y = y_j | X = x_i) p(X = x_i)$$

Independence

Marginal: P satisfies $(\mathbf{X} \perp \mathbf{Y})$ if and only if

$$P(\mathbf{X=x},\mathbf{Y=y}) = P(\mathbf{X=x})\, P(\mathbf{Y=y}),$$
$$\forall \mathbf{x} \in Val(\mathbf{X}),\ \mathbf{y} \in Val(\mathbf{Y})$$

Conditional: P satisfies $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z})$ if and only if

$$P(\mathbf{X},\mathbf{Y}|\mathbf{Z}) = P(\mathbf{X}|\mathbf{Z})\, P(\mathbf{Y}|\mathbf{Z}),$$
$$\forall \mathbf{x} \in Val(\mathbf{X}),\ \mathbf{y} \in Val(\mathbf{Y}),\ \mathbf{z} \in Val(\mathbf{Z})$$

Bayes' Theorem

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

$$p(X) = \sum_Y p(X|Y)p(Y)$$

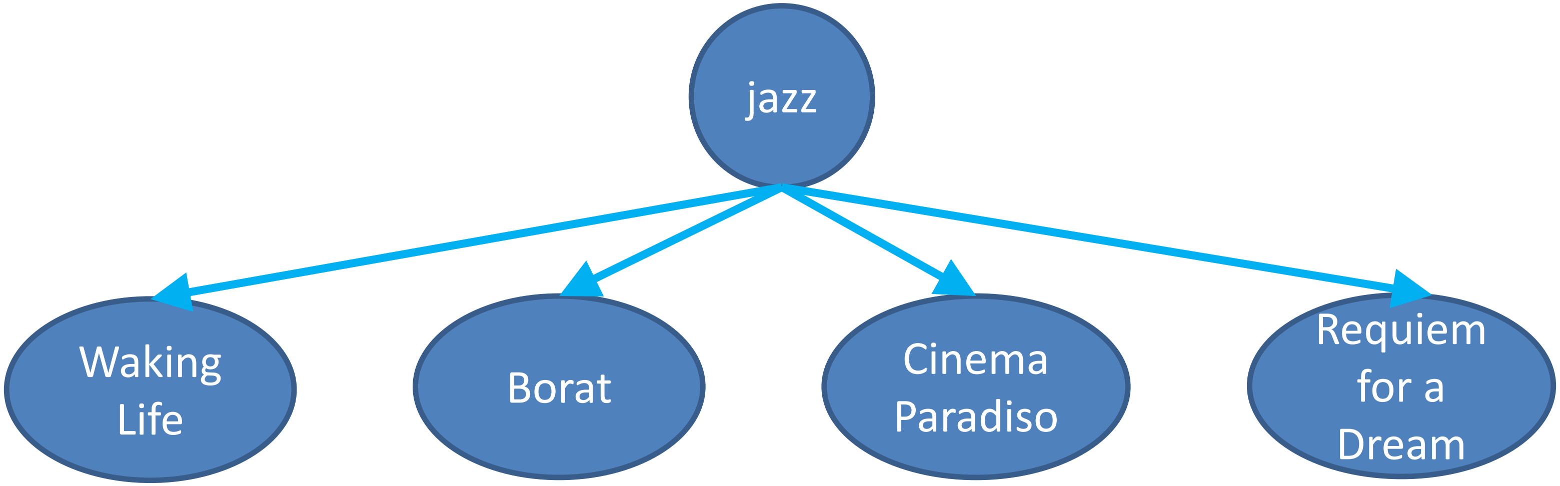
Probabilistic Graphical Models

- It is sometimes desirable to have not only a prediction y given features $\boldsymbol{x}$, but a measure of confidence $P(y|\boldsymbol{x})$
- Let $\boldsymbol{x}$ be a d-dim vector, each dim can take 2 values
- For each such vector $\boldsymbol{x}$, y=1 or y=0
- We need statistics about how frequently y=1 occurs with each of 2^d possible feature vectors → 2^d parameters to estimate
- Thus we require an unrealistic amount of data to estimate parameters (probabilities); graphical models allow simplifying assumptions

A simple alternative: Naïve Bayes

- Assume all features are independent given the class i.e. $P(\mathbf{x}|y) = \Pi_d P(x_d|y)$
- Model $P(x_d=1|y=1)$ and $P(x_d=1|y=0)$, for all d → 2d parameters (as opposed to 2^d)
- Then use Bayes rule to compute $P(y|\mathbf{x}) = P(\mathbf{x}|y) P(y) / Z = \Pi_d P(x_d|y) P(y) / Z$
- Where Z is a normalizing constant

Naïve Bayes example



If J=1	Prob W=1	Prob B=1	Prob C=1	Prob R=1
True	0.8	0.2	0.7	0.5
False	0.3	0.5	0.3	0.4

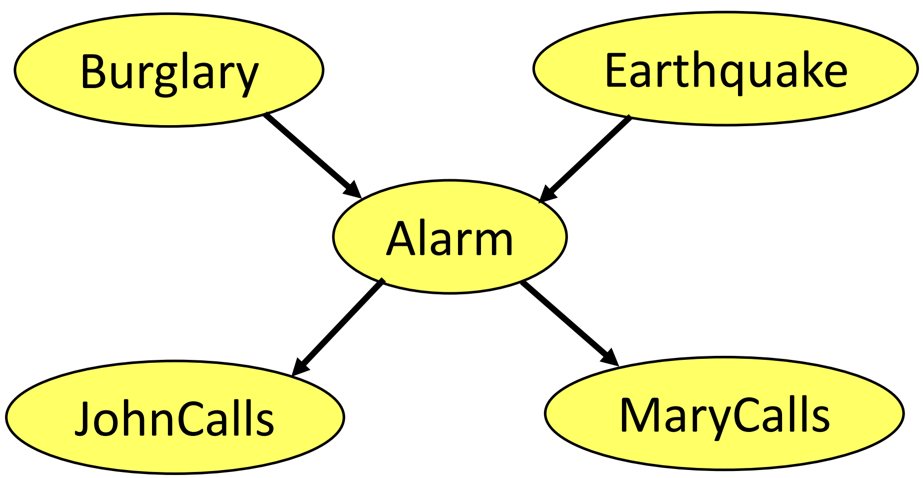
Advantages of Graphical Models

- If no assumption of independence is made, must estimate an exponential number of parameters
- If we assume all variables independent, efficient training and inference possible, but assumption too strong
- **Graphical models** use **graphs** over random variables to specify variable **dependencies (relationships)**
  - Allows for less restrictive independence assumptions while limiting the number of parameters that must be estimated
  - Allows some interpretability
  - **Bayesian networks**: **Directed** acyclic graphs indicate causal structure
  - **Markov networks**: **Undirected** graphs capture general dependencies

Adapted from Ray Mooney

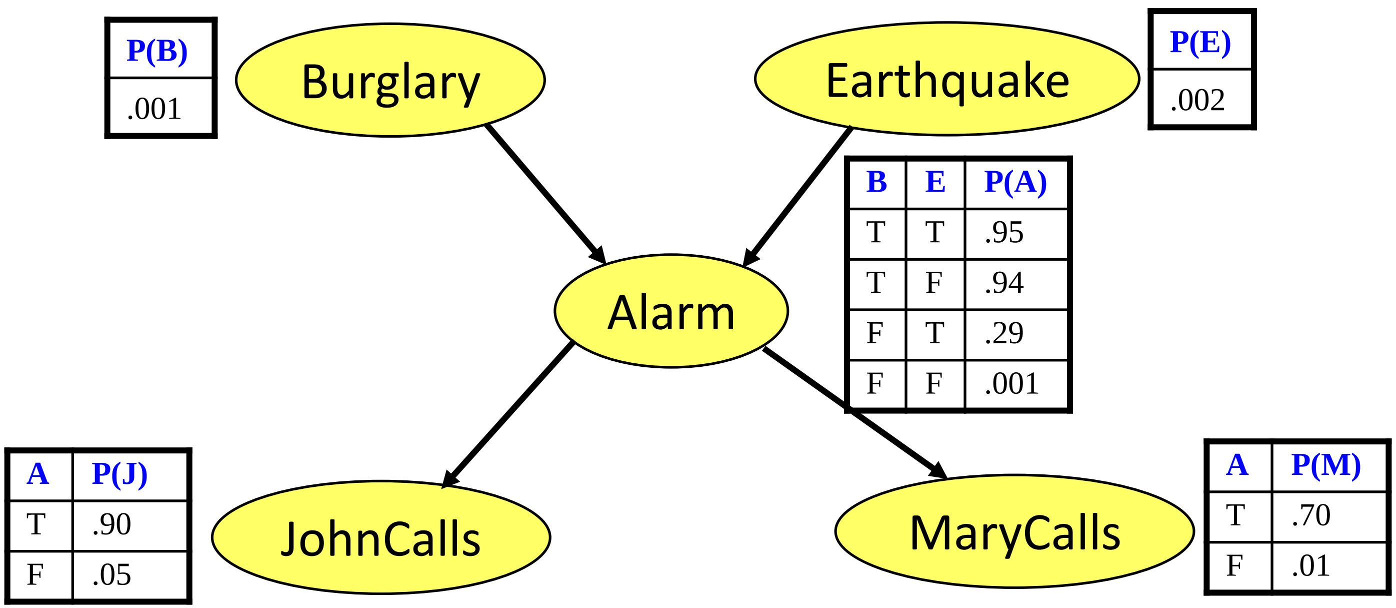
Bayesian Networks

- Directed Acyclic Graph (DAG)
- Nodes are random variables
- Edges indicate causal influences



Conditional Probability Tables

- Each node has a **conditional probability table** (**CPT**) that gives the probability of each of its values given every possible combination of values for its parents
  - Roots of the DAG that have no parents are given prior probabilities



P(B)
.001

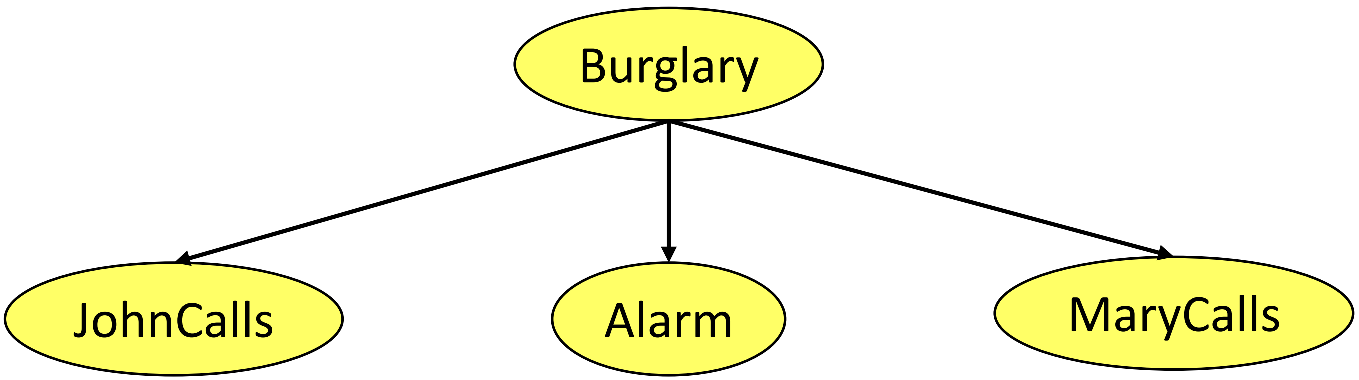
P(E)
.002

B	E	P(A)
T	T	.95
T	F	.94
F	T	.29
F	F	.001

A	P(J)
T	.90
F	.05

A	P(M)
T	.70
F	.01

Aside: Naïve Bayes version

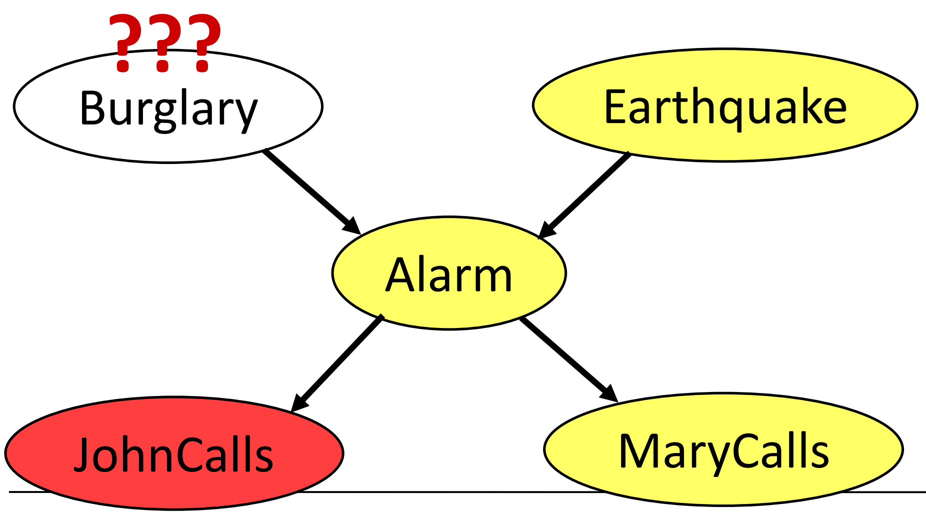


CPT Comments

- Probability of false not given since rows must add to 1
- Example requires 10 parameters rather than 2^5–1=31 for specifying the full joint distribution
- Number of parameters in the CPT for a node is exponential in the number of parents

Bayes Net Inference

- Given known values for some **evidence variables**, determine the posterior probability of some **query variables**
- Example: Given that John calls, what is the probability that there is a Burglary?

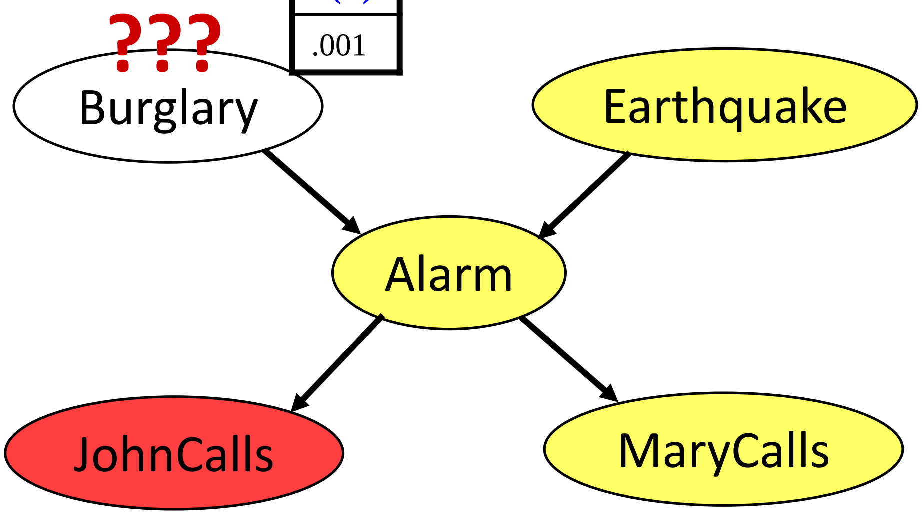


John calls 90% of the time there is an Alarm and the Alarm detects 94% of Burglaries so people generally think it should be fairly high.

However, this ignores the prior probability of John calling.

Bayes Net Inference

- Example: Given that John calls, what is the probability that there is a Burglary?



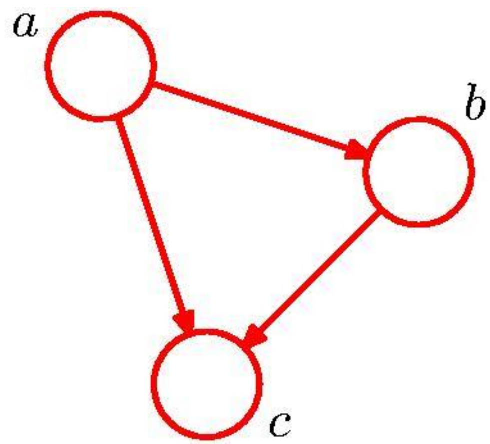
P(B)
.001

A	P(J)
T	.90
F	.05

John also calls 5% of the time when there is no Alarm. So over 1,000 days we expect 1 Burglary and John will probably call. However, he will also call with a false report 50 times on average. So the call is about 50 times more likely a false report: P(Burglary | JohnCalls) ≈ 0.02

Bayes Nets (not yet useful)

- No independence encoded



$$p(x_1, \ldots, x_K) = p(x_K | x_1, \ldots, x_{K-1}) \ldots p(x_2 | x_1) p(x_1)$$

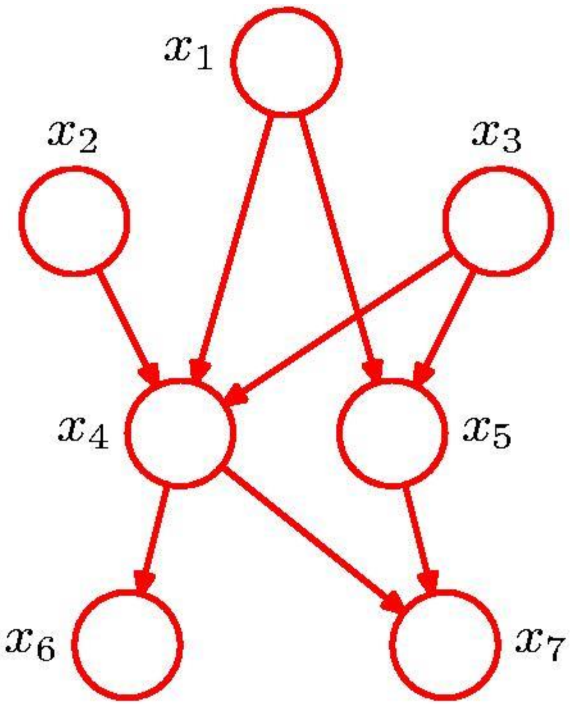
$$p(a, b, c) = p(c|a, b) p(a, b) = p(c|a, b) p(b|a) p(a)$$

Chris Bishop

Bayes Nets (formulation)

- More interesting: Some independences encoded

$p(x_1, \ldots, x_7)$



General Factorization

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$

Conditional Independence

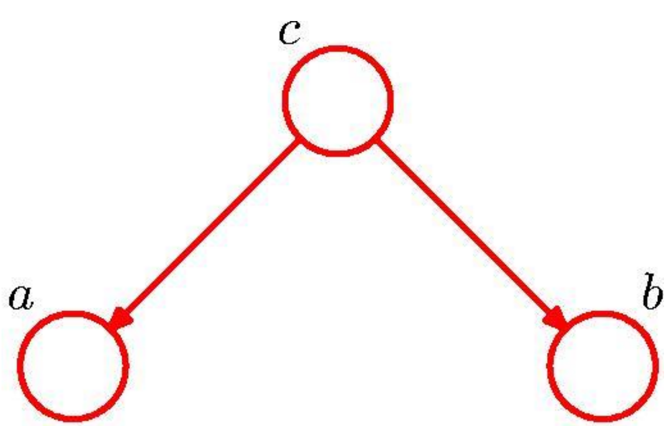
a is independent of b given c

$$p(a|b,c) = p(a|c)$$

Equivalently
$$\begin{aligned} p(a,b|c) &= p(a|b,c)p(b|c) \\ &= p(a|c)p(b|c) \end{aligned}$$

Notation
$$a \perp\!\!\!\perp b \mid c$$

Conditional Independence: Example 1



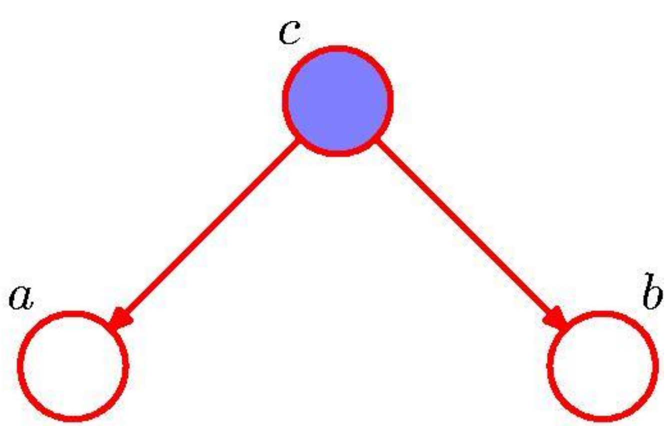
$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

$$p(a, b) = \sum_c p(a|c)p(b|c)p(c)$$

$$a \not\perp\!\!\!\perp b \mid \emptyset$$

Node *c* is “tail to tail” for path from *a* to *b*:
No independence of *a* and *b* follows from this path

Conditional Independence: Example 1



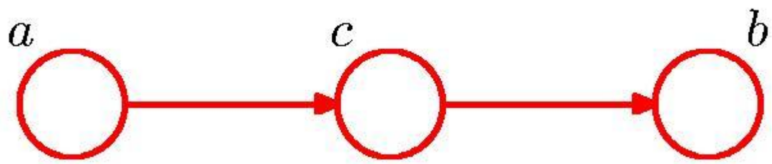
$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

$$\begin{aligned} p(a, b|c) &= \frac{p(a, b, c)}{p(c)} \\ &= p(a|c)p(b|c) \end{aligned}$$

$$a \perp\!\!\!\perp b \mid c$$

Node *c* is "tail to tail" for path from *a* to *b*:
Observing *c* blocks the path thus making *a* and *b* **conditionally independent**

Conditional Independence: Example 2



$$p(a,b,c) = p(a)p(c|a)p(b|c)$$

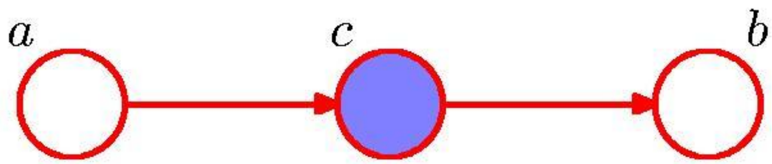
$$p(a,b) = p(a)\sum_c p(c|a)p(b|c) = p(a)p(b|a)$$

$$a \not\perp\!\!\!\perp b \mid \emptyset$$

Σ_c p(c|a) p(b|c) =
Σ_c p(c|a) **p(b|c, a)** = // next slide
Σ_c p(b, c|a) =
p(b|a)

Node *c* is "head to tail" for path from *a* to *b*:
No independence of *a* and *b* follows from this path

Conditional Independence: Example 2

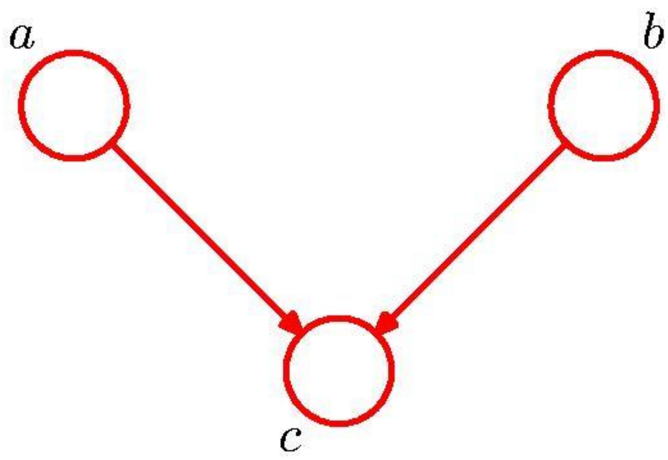


$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(c|a)p(b|c)}{p(c)} = p(a|c)p(b|c)$$

$$a \perp\!\!\!\perp b \mid c$$

Node *c* is “head to tail” for path from *a* to *b*:
Observing *c* blocks the path thus making *a* and *b* **conditionally independent**

Conditional Independence: Example 3



$$p(a,b,c) = p(a)p(b)p(c|a,b)$$

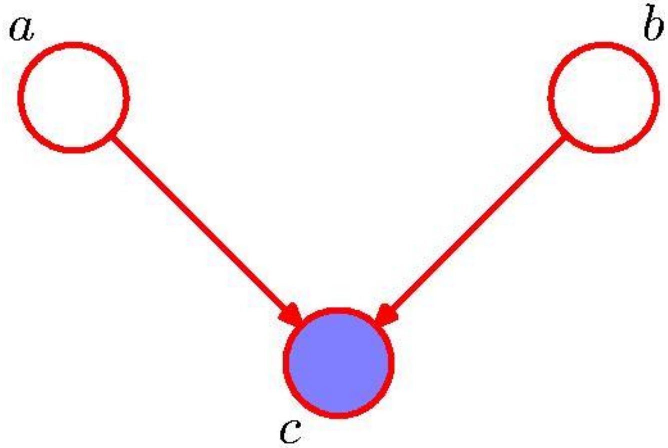
$$p(a,b) = p(a)p(b)$$

$$a \perp\!\!\!\perp b \mid \emptyset$$

Node *c* is **"head to head"** for path from *a* to *b*:
Unobserved *c* blocks the path thus making *a* and *b* **independent**

Note: this is the opposite of Example 1, with c unobserved.

Conditional Independence: Example 3



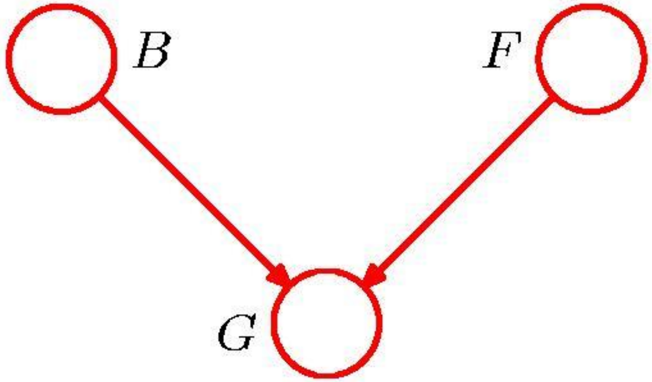
$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(b)p(c|a,b)}{p(c)}$$

$$a \not\perp\!\!\!\perp b \mid c$$

Node *c* is **"head to head"** for path from *a* to *b*:
Observing *c* **unblocks** the path thus making *a* and *b* **conditionally dependent**

Note: this is the opposite of Example 1, with c observed.

Example: “Am I out of fuel?”



$$
\begin{aligned}
p(G=1|B=1,F=1) &= 0.8\\
p(G=1|B=1,F=0) &= 0.2\\
p(G=1|B=0,F=1) &= 0.2\\
p(G=1|B=0,F=0) &= 0.1
\end{aligned}
$$

B = Battery (0=flat, 1=fully charged)
F = Fuel Tank (0=empty, 1=full)
G = Fuel Gauge Reading (0=empty, 1=full)

$$
\begin{aligned}
p(B=1) &= 0.9\\
p(F=1) &= 0.9
\end{aligned}
$$

and hence

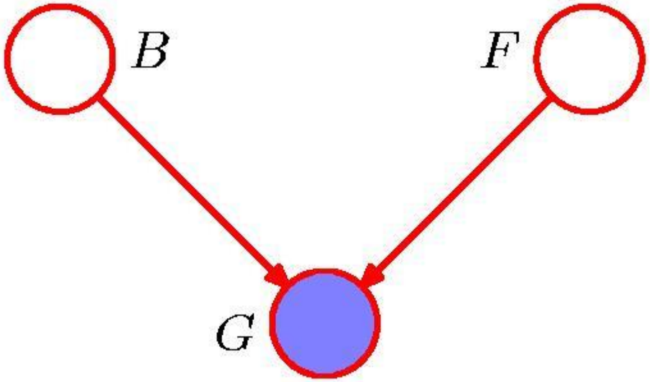
$$p(F=0) = 0.1$$

Example: “Am I out of fuel?”

$$p(G=0|F=0) = \sum_{B\in\{0,1\}} p(G=0|B,F=0)p(B) = 0.81$$

$$p(F=0) \quad = \quad 0.1$$

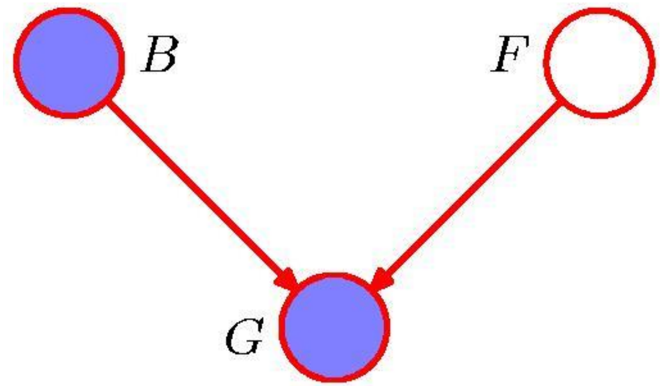
$$p(G=0) = \sum_{B\in\{0,1\}} \sum_{F\in\{0,1\}} p(G=0|B,F)p(B)p(F) = 0.315$$



$$\begin{aligned} p(F=0|G=0) &= \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \\ &\simeq 0.257 \end{aligned}$$

Probability of an empty tank increased by observing $G=0$.

Example: “Am I out of fuel?”



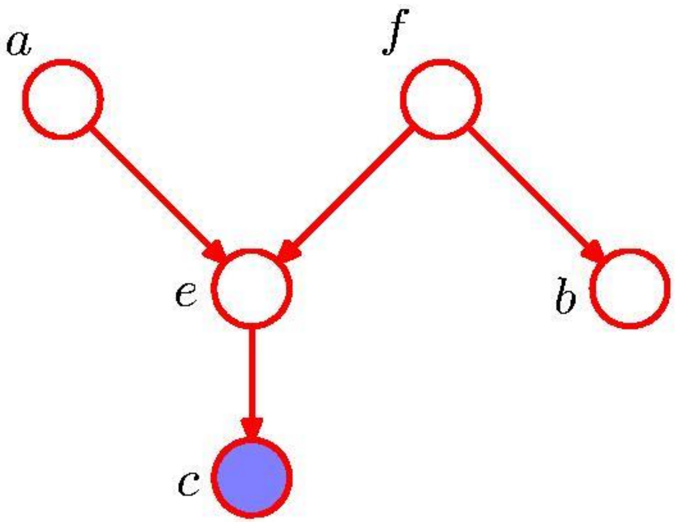
$$p(F=0|G=0,B=0) = \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \simeq 0.111$$

Probability of an empty tank reduced by observing $B=0$.
This is referred to as “explaining away”.

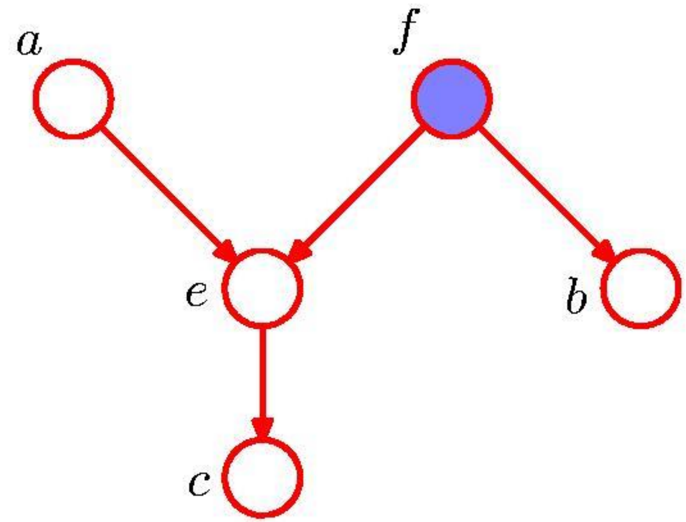
D-separation

- A, B, and C are non-intersecting subsets of nodes in a directed graph.
- A path from A to B is blocked if it contains a node such that either
  a) the arrows on the path meet either head-to-tail or tail-to-tail at the node, and the node is in the set C, or
  b) the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, are in the set C.
- If all paths from A to B are blocked, A is said to be d-separated from B by C.
- If A is d-separated from B by C, the joint distribution over all variables in the graph satisfies $A \perp\!\!\!\perp B \mid C$.

D-separation: Example



$$a \not\perp\!\!\!\perp b \mid c$$



$$a \perp\!\!\!\perp b \mid f$$

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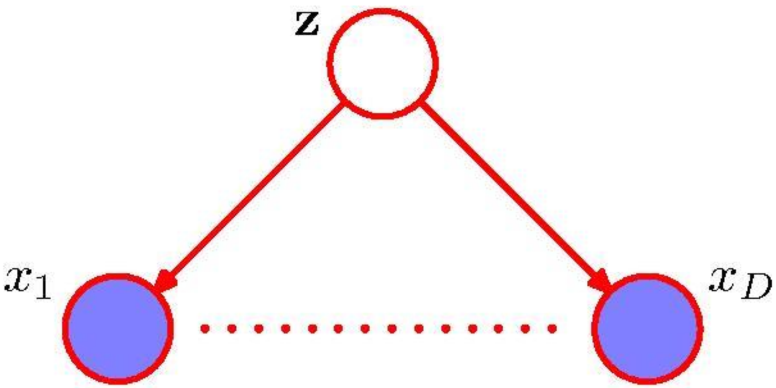
Naïve Bayes



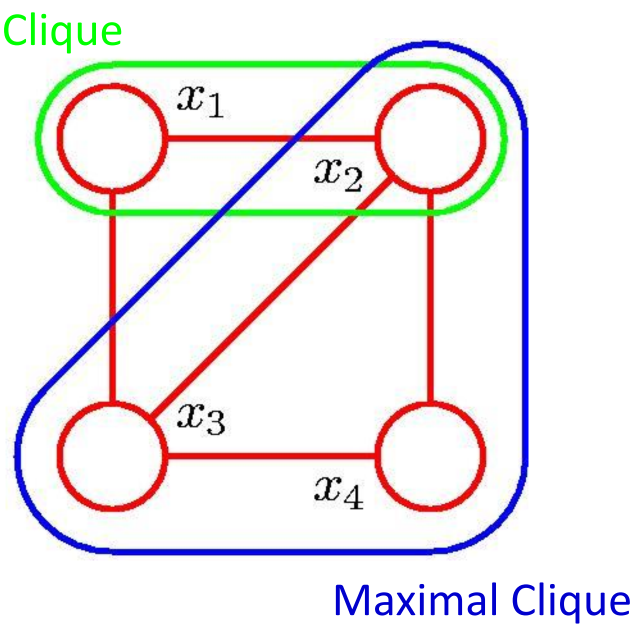
Conditioned on the class **z**,
the distributions of the input variables $x_1, \ldots, x_D$ are independent.

Are the $x_1, \ldots, x_D$ marginally independent?

Bayes Nets vs. Markov Nets

- Bayes nets represent a subclass of joint distributions that capture non-cyclic *causal* dependencies between variables.
- A Markov net can represent any joint distribution.

Cliques and Maximal Cliques



Joint Distribution for a Markov Net

- The distribution of a Markov net is described in terms of a set of **potential functions**, ψ_C, for each clique C in the graph.
- For each joint assignment of values to the variables in clique C, ψ_C assigns a non-negative real value that represents the compatibility of these values.

Joint Distribution for a Markov Net

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C} \psi_C(\mathbf{x}_C)$$

where $\psi_C(\mathbf{x}_C)$ is the potential over clique C and

$$Z = \sum_{\mathbf{x}} \prod_{C} \psi_C(\mathbf{x}_C)$$

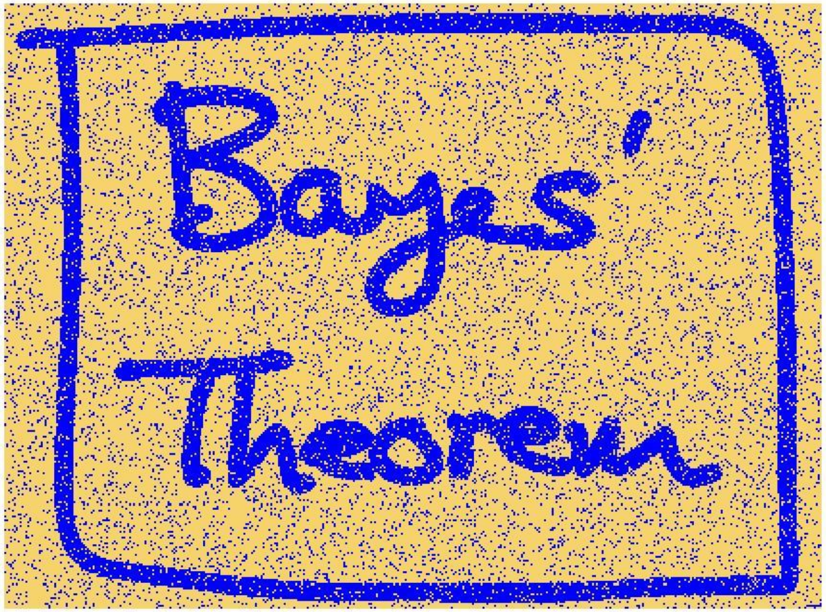
is the normalization coefficient; note: M K-state variables $\rightarrow K^M$ terms in Z.

Energies and the Boltzmann distribution

$$\psi_C(\mathbf{x}_C) = \exp\left\{-E(\mathbf{x}_C)\right\}$$

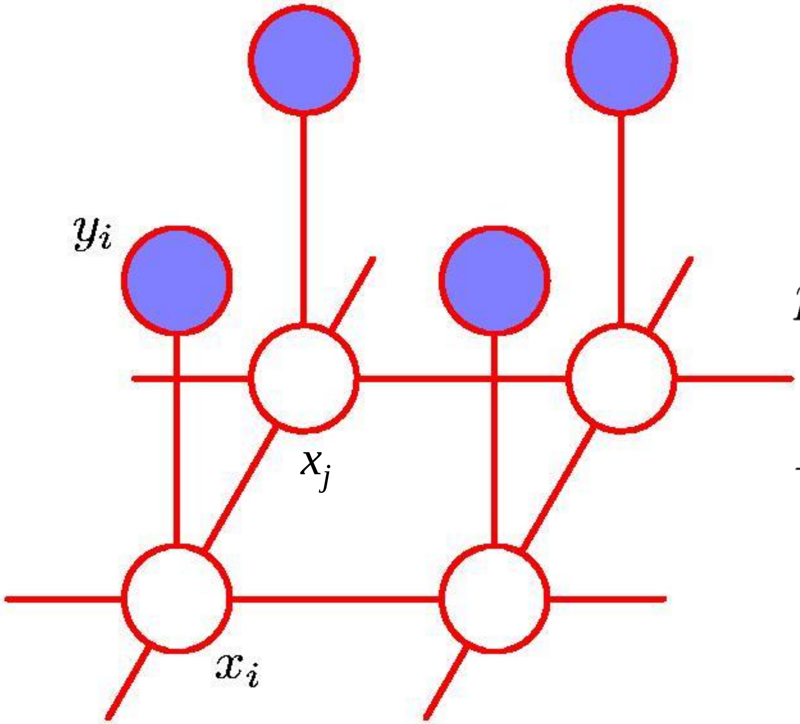
Illustration: Image De-Noising

Original Image



Noisy Image

Illustration: Image De-Noising



y_i in {+1, -1}: labels in noisy image (which we have),
x_i in {+1, -1}: labels in noise-free image (which we want to recover),
i is the index over pixels

$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\{-E(\mathbf{x}, \mathbf{y})\}$$

$$E(\mathbf{x}, \mathbf{y}) = h \sum_i x_i - \beta \sum_{\{i,j\}} x_i x_j - \eta \sum_i x_i y_i$$

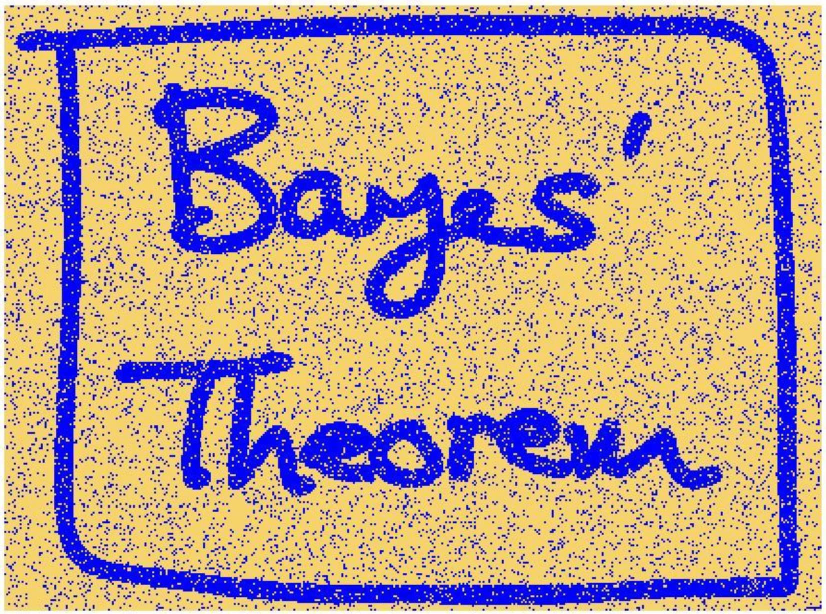
Prior

Pixels are like their neighbors

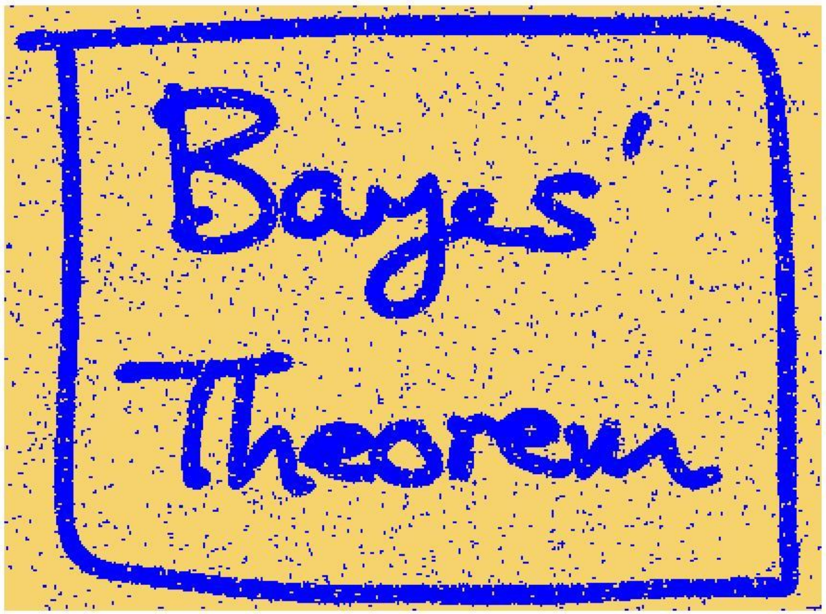
Pixels of noisy and noise-free images are related

Adapted from Chris Bishop

Illustration: Image De-Noising



Noisy Image



Restored Image (ICM)

Aside: Graphical vs other models

- Some graphical models are generative i.e. model p(x) not just p(y|x)
- Consider relationships of the features
- Somewhat interpretable
- We'll also discuss one model appropriate for sequence classification (e.g. weather)

Classifying Connected Samples (Sequences)

- Standard classification problem assumes individual cases are disconnected and independent (i.i.d.: independently and identically distributed).
- Many problems do not satisfy this assumption and involve making many connected decisions which are mutually dependent.

Markov Chains

- A finite state machine with probabilistic state transitions.
- Makes Markov assumption that next state only depends on the current state and independent of previous history.

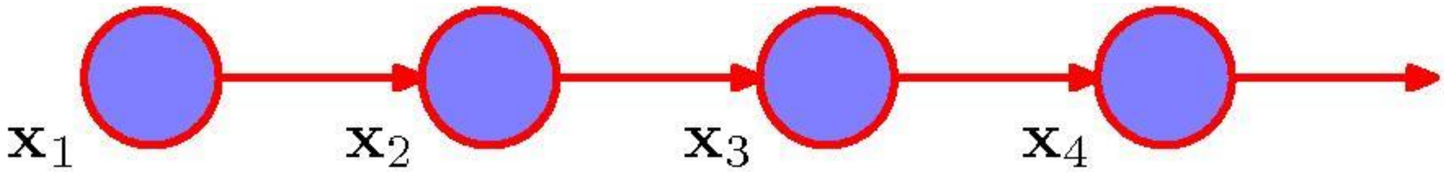
Markov Chains

- General joint probability distribution:

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{x}_1, \ldots, \mathbf{x}_{n-1})$$

- First-order Markov chain:

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_N) = p(\mathbf{x}_1) \prod_{n=2}^{N} p(\mathbf{x}_n | \mathbf{x}_{n-1})$$

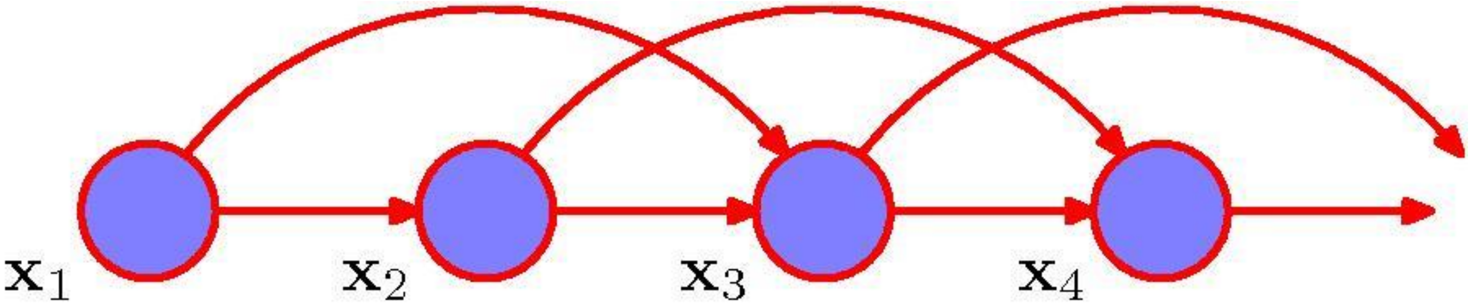


Figures from Chris Bishop

Markov Chains

- Second-order Markov chain:

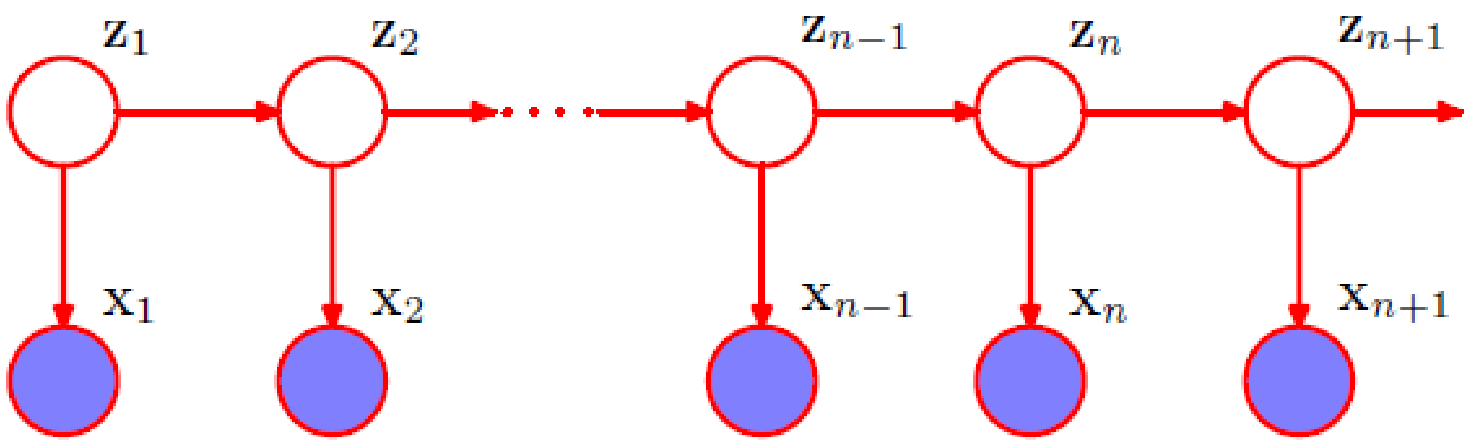
$$p(\mathbf{x}_1, \ldots, \mathbf{x}_N) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1) \prod_{n=3}^{N} p(\mathbf{x}_n|\mathbf{x}_{n-1}, \mathbf{x}_{n-2})$$



Figures from Chris Bishop

Hidden Markov Models

- Latent variables (**z**) satisfy Markov property
- Observed variables/predictions (**x**) *do not*
- Example: **x** = words, **z** = parts of speech



$$p(\mathbf{x}_1,\ldots,\mathbf{x}_N,\mathbf{z}_1,\ldots,\mathbf{z}_N) = p(\mathbf{z}_1)\left[\prod_{n=2}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1})\right]\prod_{n=1}^{N} p(\mathbf{x}_n|\mathbf{z}_n)$$

Figures from Chris Bishop

Example: Part Of Speech Tagging

- Annotate each word in a sentence with a part-of-speech marker.

John	saw	the	saw	and	decided	to	take	it	to	the	table.
NNP	VBD	DT	NN	CC	VBD	TO	VB	PRP	IN	DT	NN

Adapted from Ray Mooney

English Parts of Speech

- Noun (person, place or thing)
  - Singular (NN): dog, fork
  - Plural (NNS): dogs, forks
  - Proper (NNP, NNPS): John, Springfields
  - Personal pronoun (PRP): I, you, he, she, it
  - Wh-pronoun (WP): who, what
- Verb (actions and processes)
  - Base, infinitive (VB): eat
  - Past tense (VBD): ate
  - Gerund (VBG): eating
  - Past participle (VBN): eaten
  - Non 3rd person singular present tense (VBP): eat
  - 3rd person singular present tense: (VBZ): eats
  - Modal (MD): should, can
  - To (TO): to (to eat)

English Parts of Speech (cont.)

- Adjective (modify nouns)
  - Basic (JJ): red, tall
  - Comparative (JJR): redder, taller
  - Superlative (JJS): reddest, tallest
- Adverb (modify verbs)
  - Basic (RB): quickly
  - Comparative (RBR): quicker
  - Superlative (RBS): quickest
- Preposition (IN): on, in, by, to, with
- Determiner:
  - Basic (DT) a, an, the
  - WH-determiner (WDT): which, that
- Coordinating Conjunction (CC): and, but, or,
- Particle (RP): off (took off), up (put up)

Ambiguity in POS Tagging

- “Like” can be a verb or a preposition
  - I like/VBP candy.
  - Time flies like/IN an arrow.
- “Around” can be a preposition, particle, or adverb
  - I bought it at the shop around/IN the corner.
  - I never got around/RP to getting a car.
  - A new Prius costs around/RB $25K.
- Context from other words can help classify

Adapted from Ray Mooney

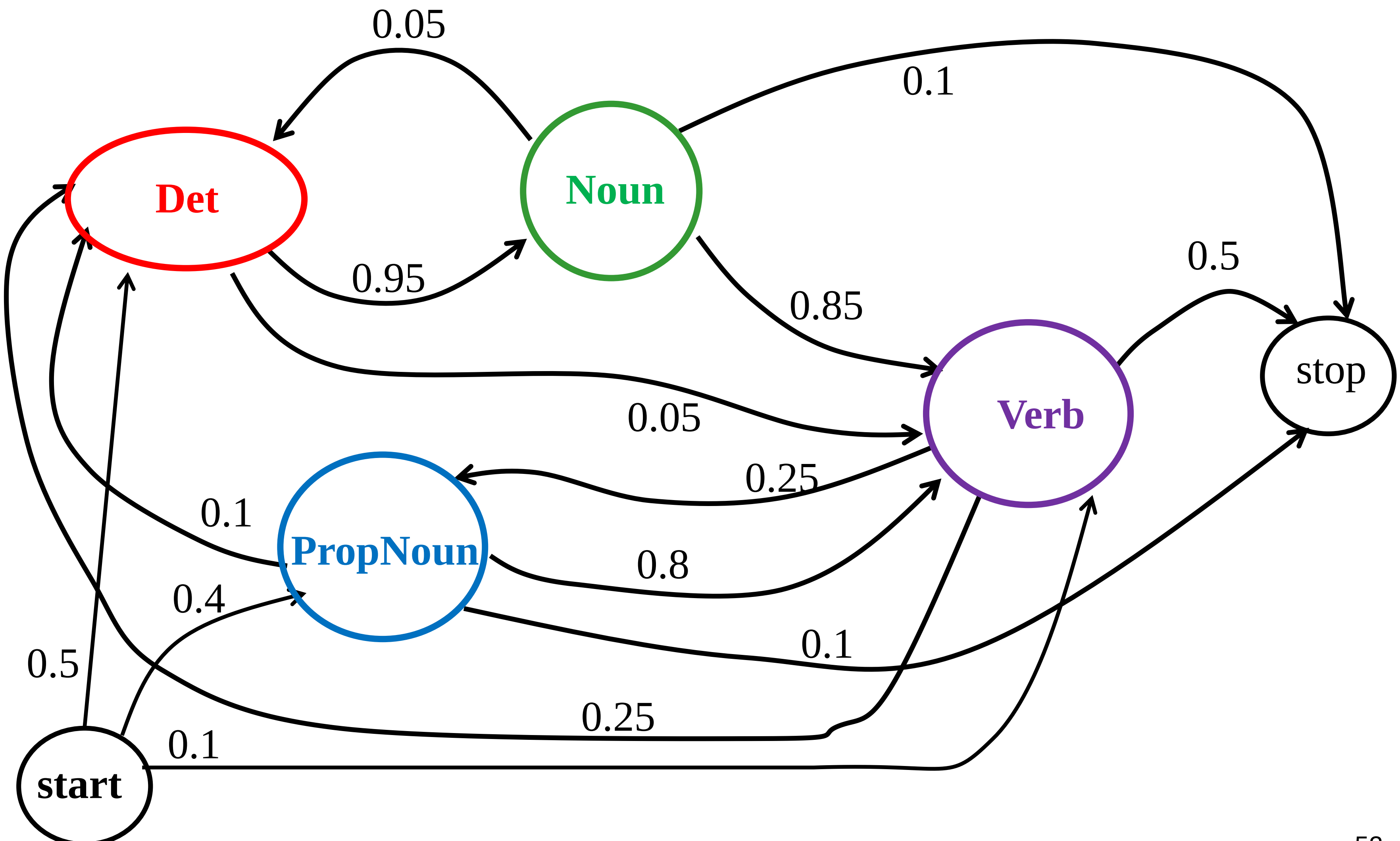
Aside: Why talking about HMMs

- A probabilistic graphical model
- Introduce sequence classification, nice way to model dynamical processes
- Introduce dealing with latent variables (not observed during training)

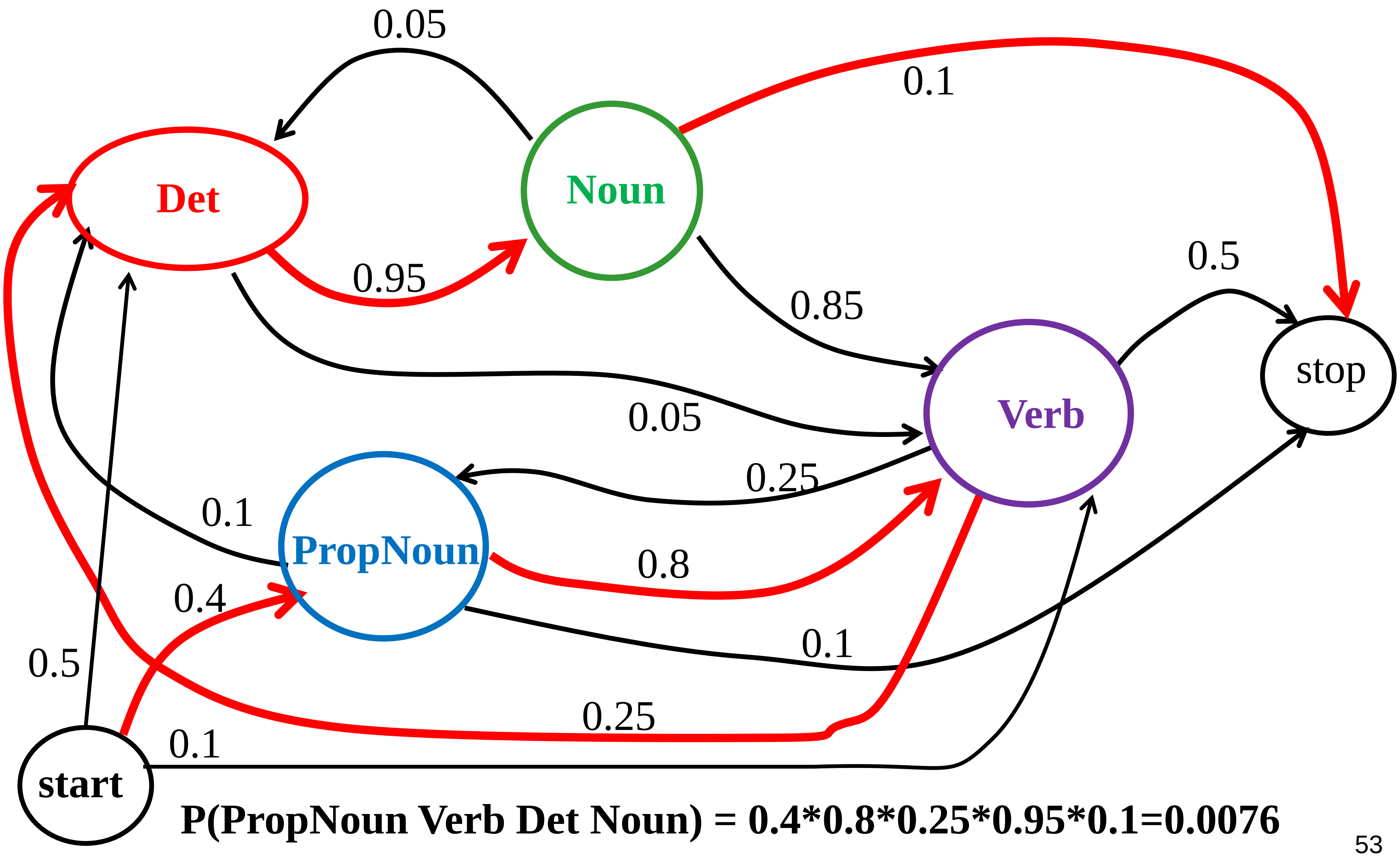
First Attempt: Markov Model

- No hidden variables
- Assume all POS are annotated by a human
- We can then reason about transitions between POS
- Goal: tag (classify) all words in a sentence with their POS

Sample Markov Model for POS



Sample Markov Model for POS

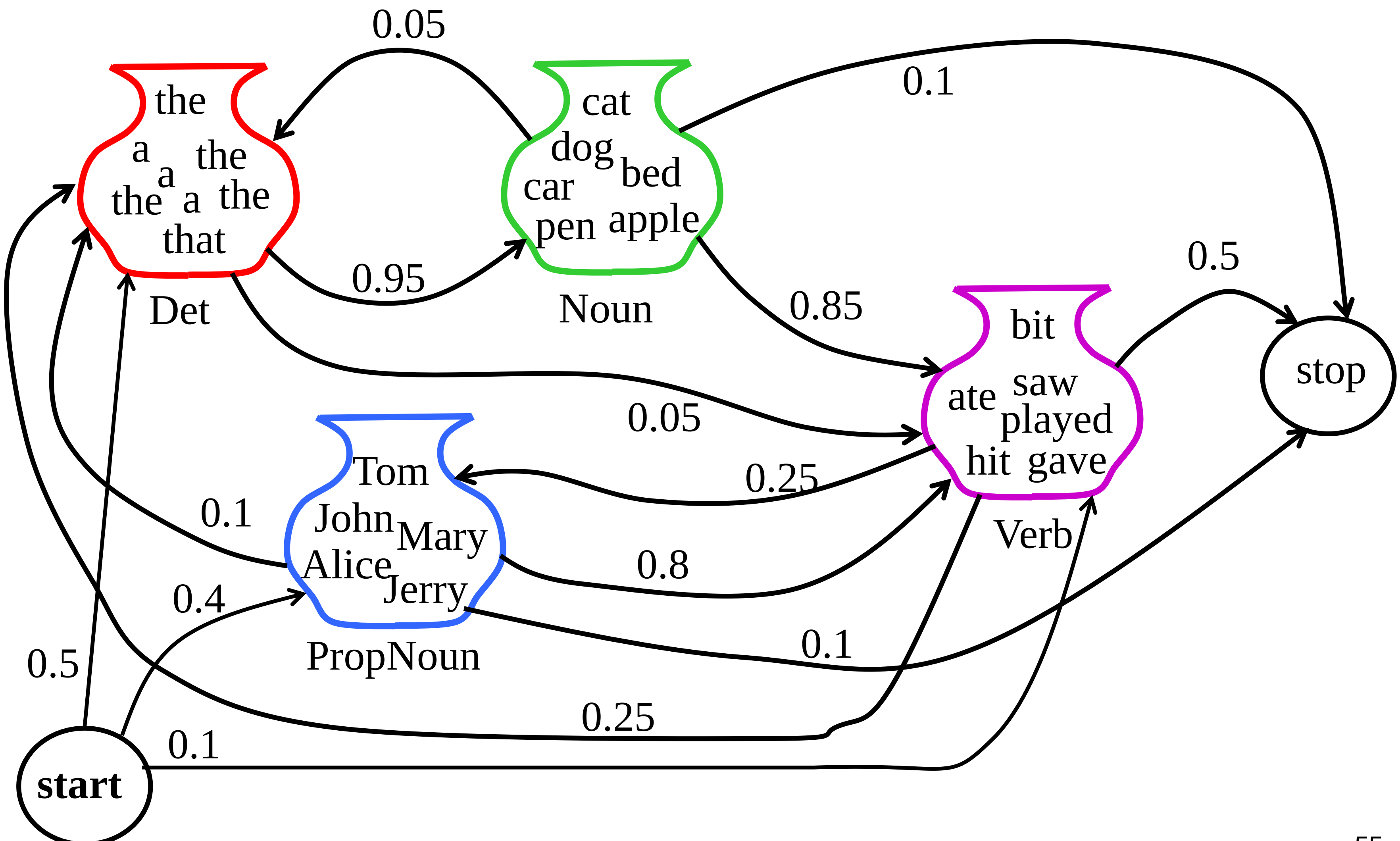


P(PropNoun Verb Det Noun) = 0.4*0.8*0.25*0.95*0.1=0.0076

Hidden Markov Models

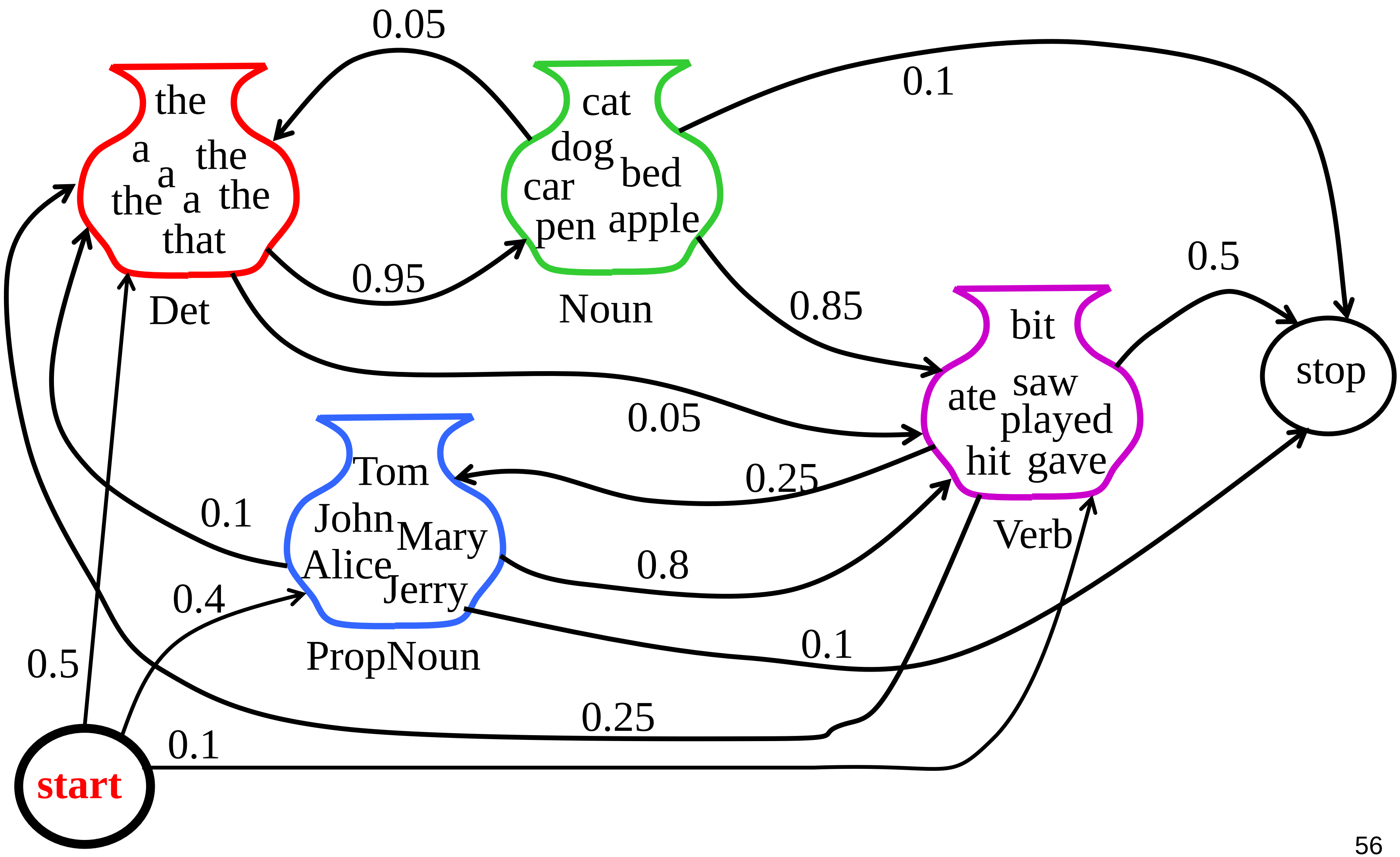
- Probabilistic generative model for sequences.
- Assume an underlying set of ***hidden*** (unobserved) states in which the model can be (e.g. parts of speech, abbreviated POS).
- Assume probabilistic transitions between states over time (e.g. transition from POS to another POS as sequence is generated).
- Assume probabilistic generation of tokens from states (e.g. words generated per POS).
- Advantages of using hidden (un-annotated) variables?

Sample HMM for POS

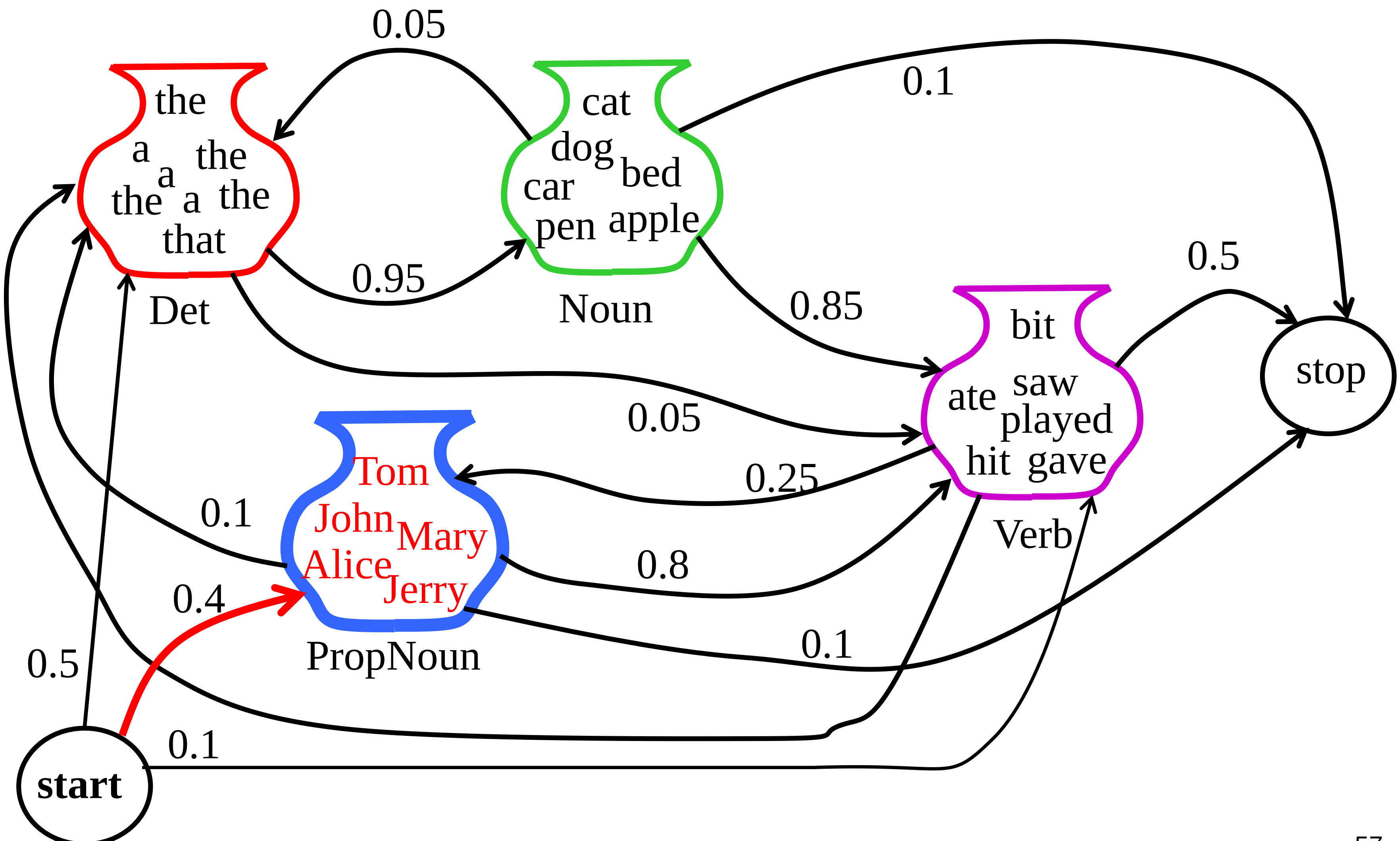


Ray Mooney

Sample HMM Generation



Sample HMM Generation



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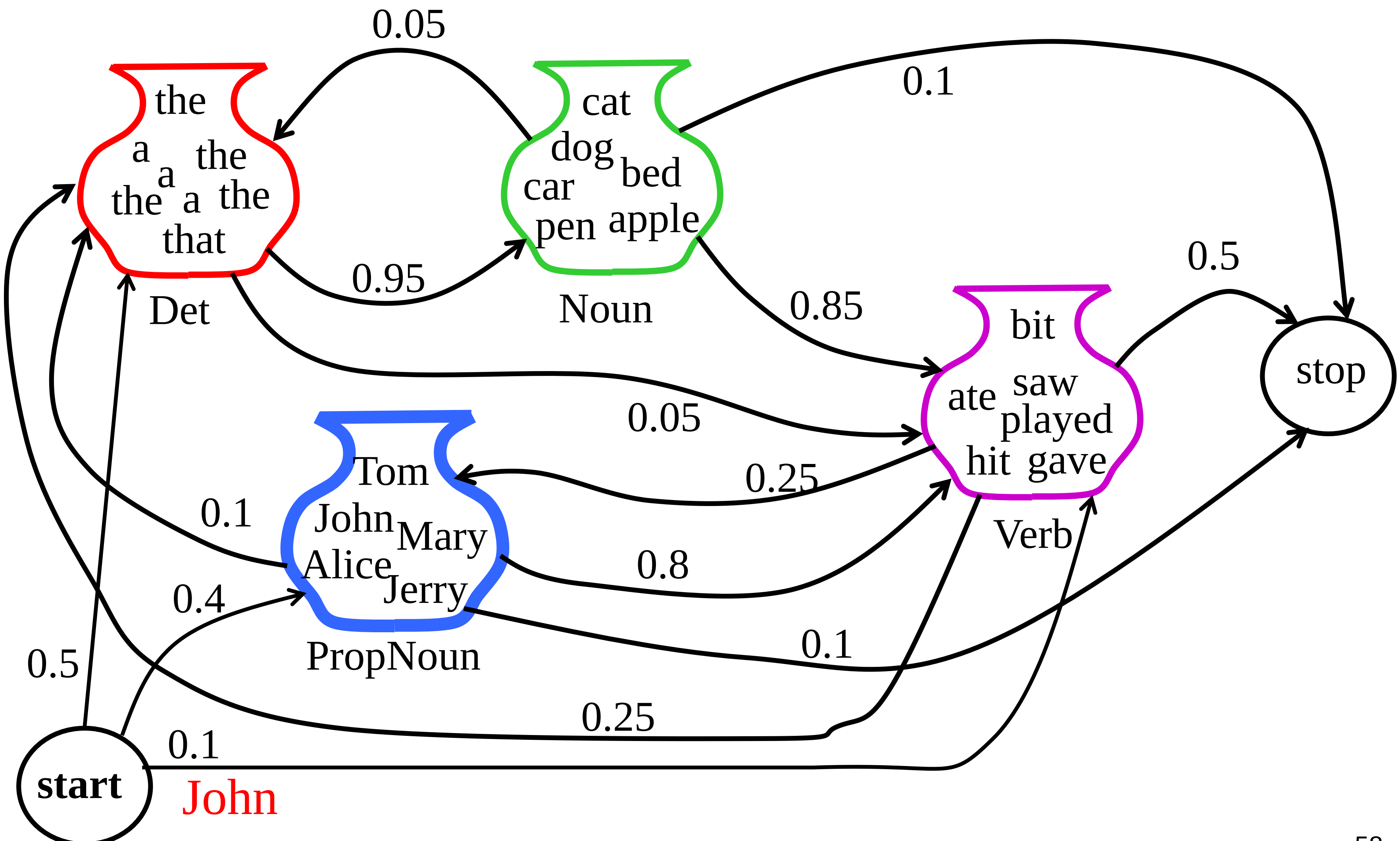
Sample HMM Generation



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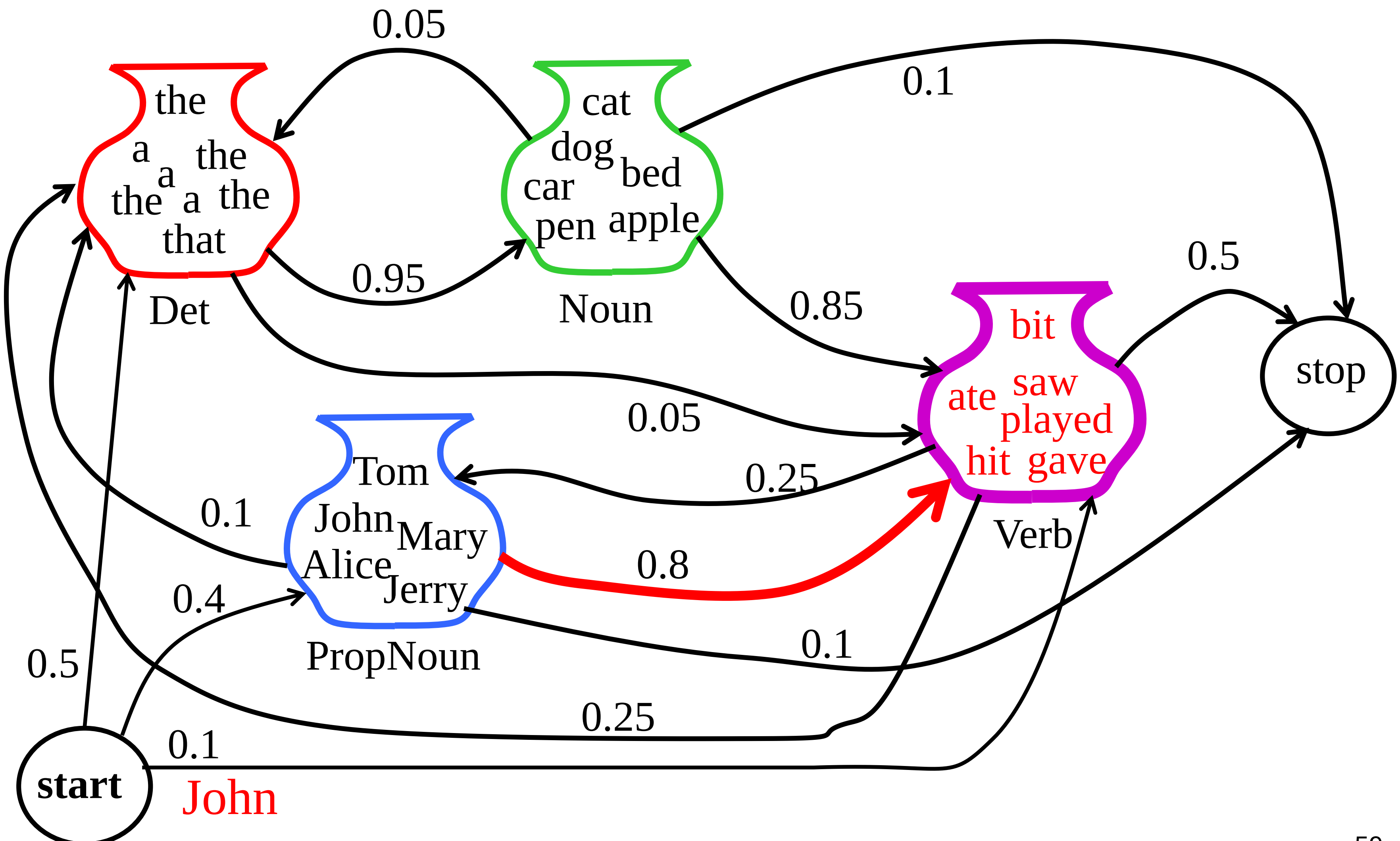
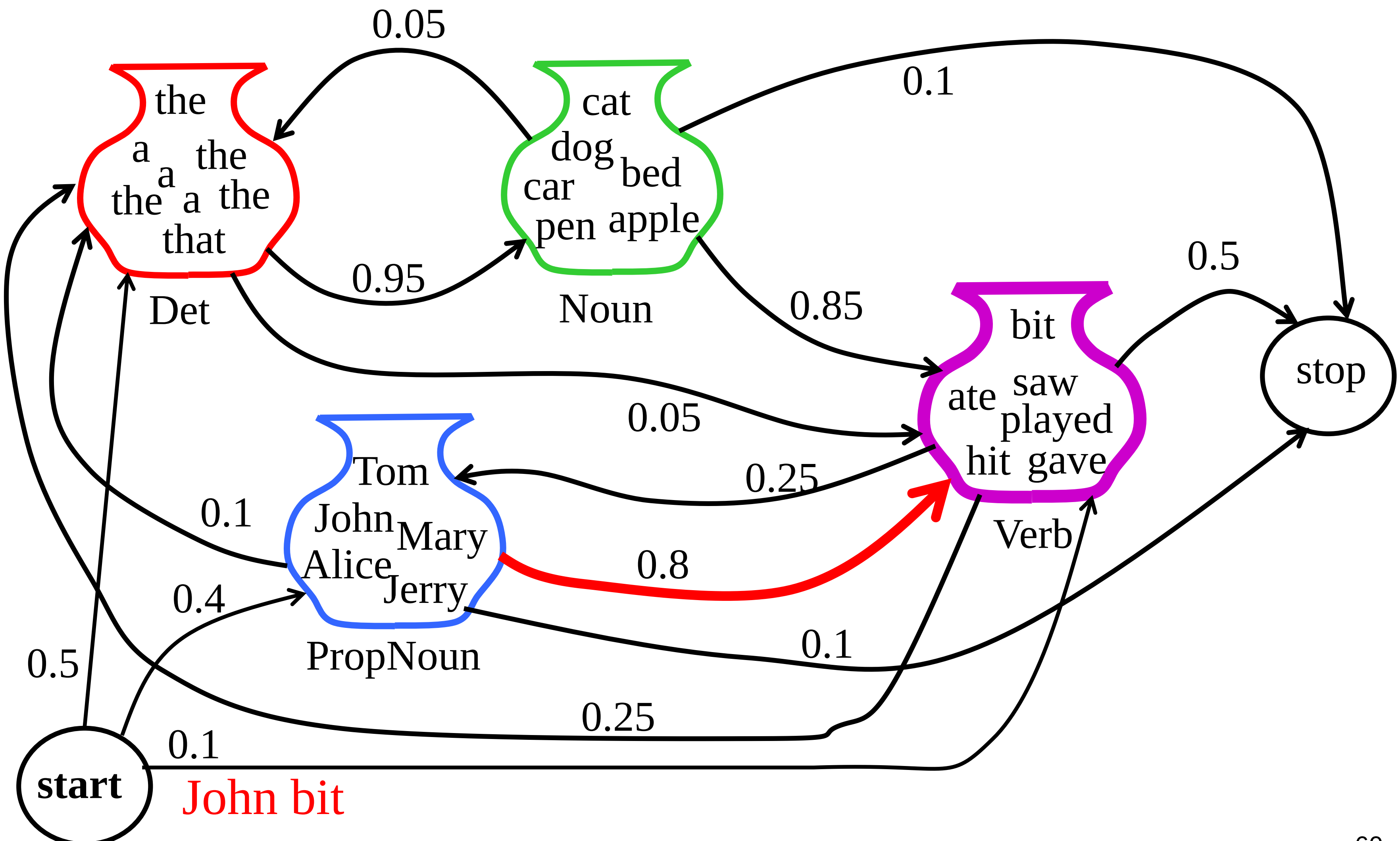
Sample HMM Generation



Sample HMM Generation



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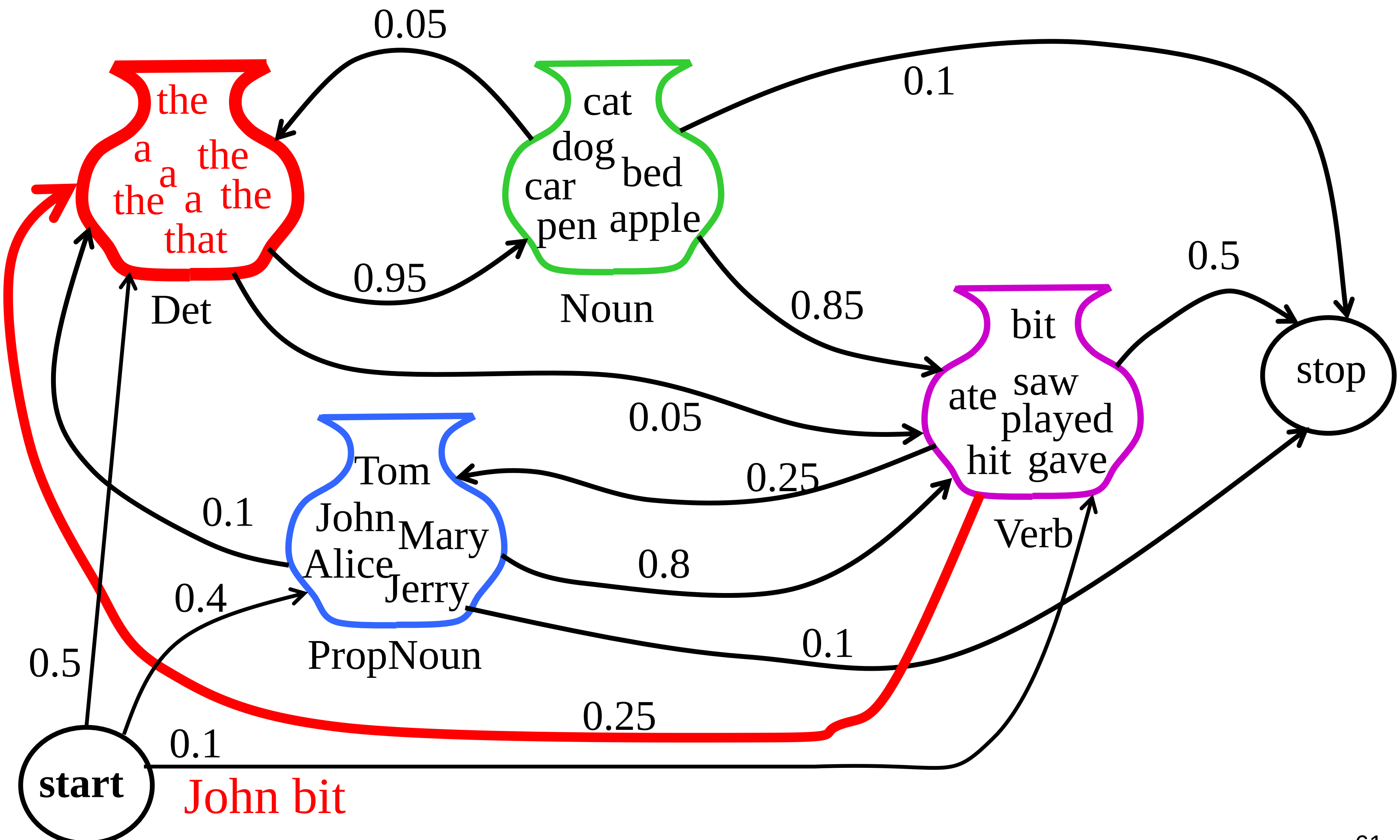
Sample HMM Generation



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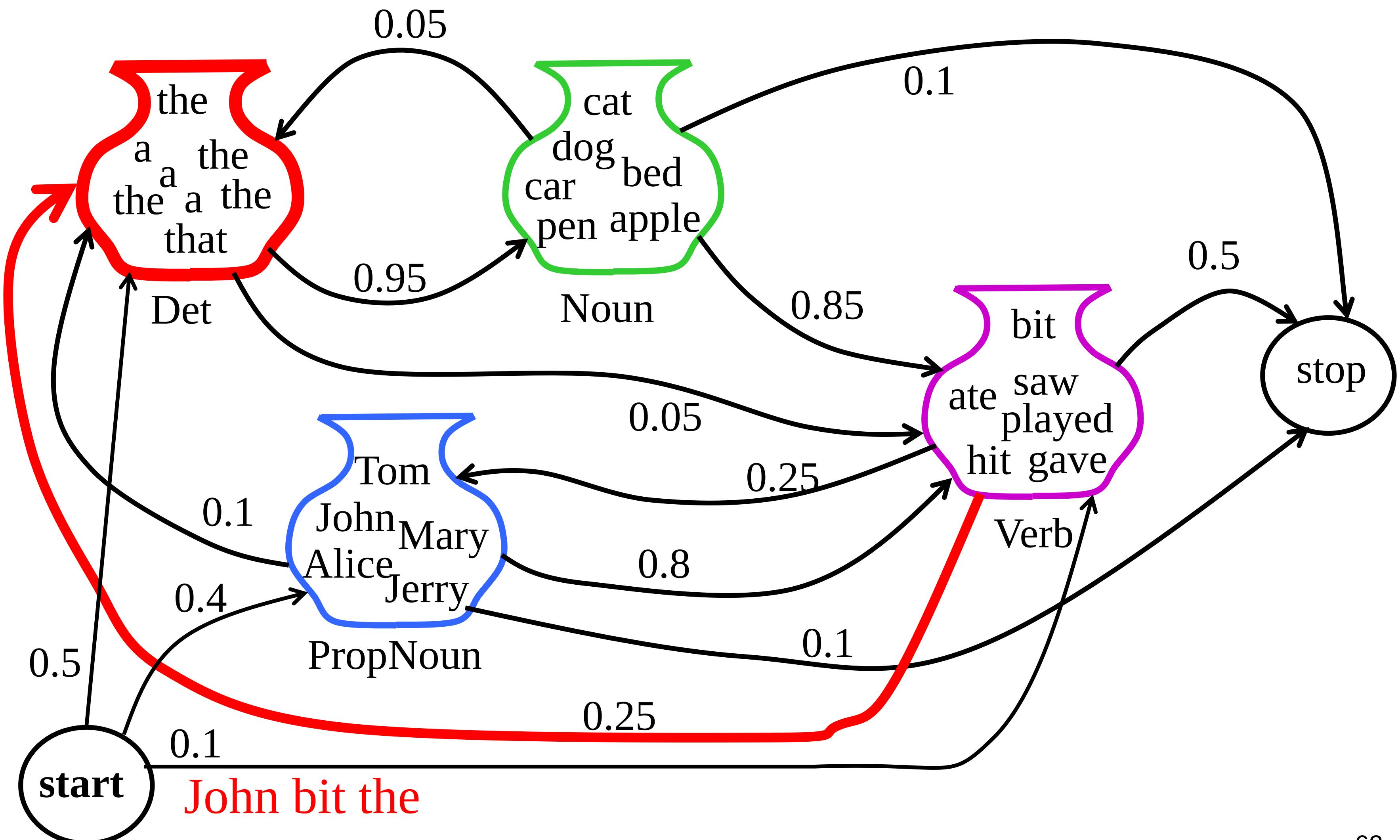
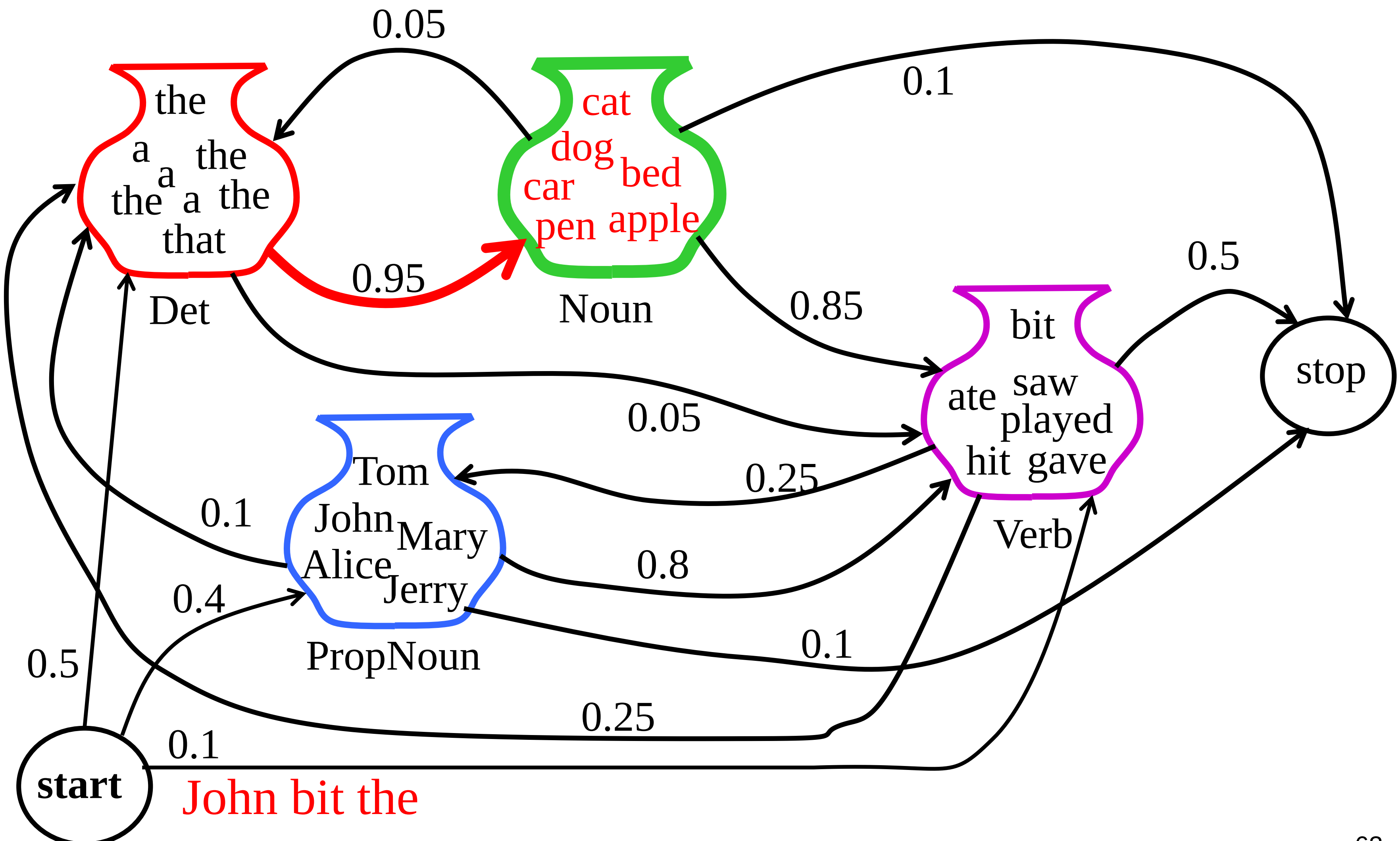
Sample HMM Generation



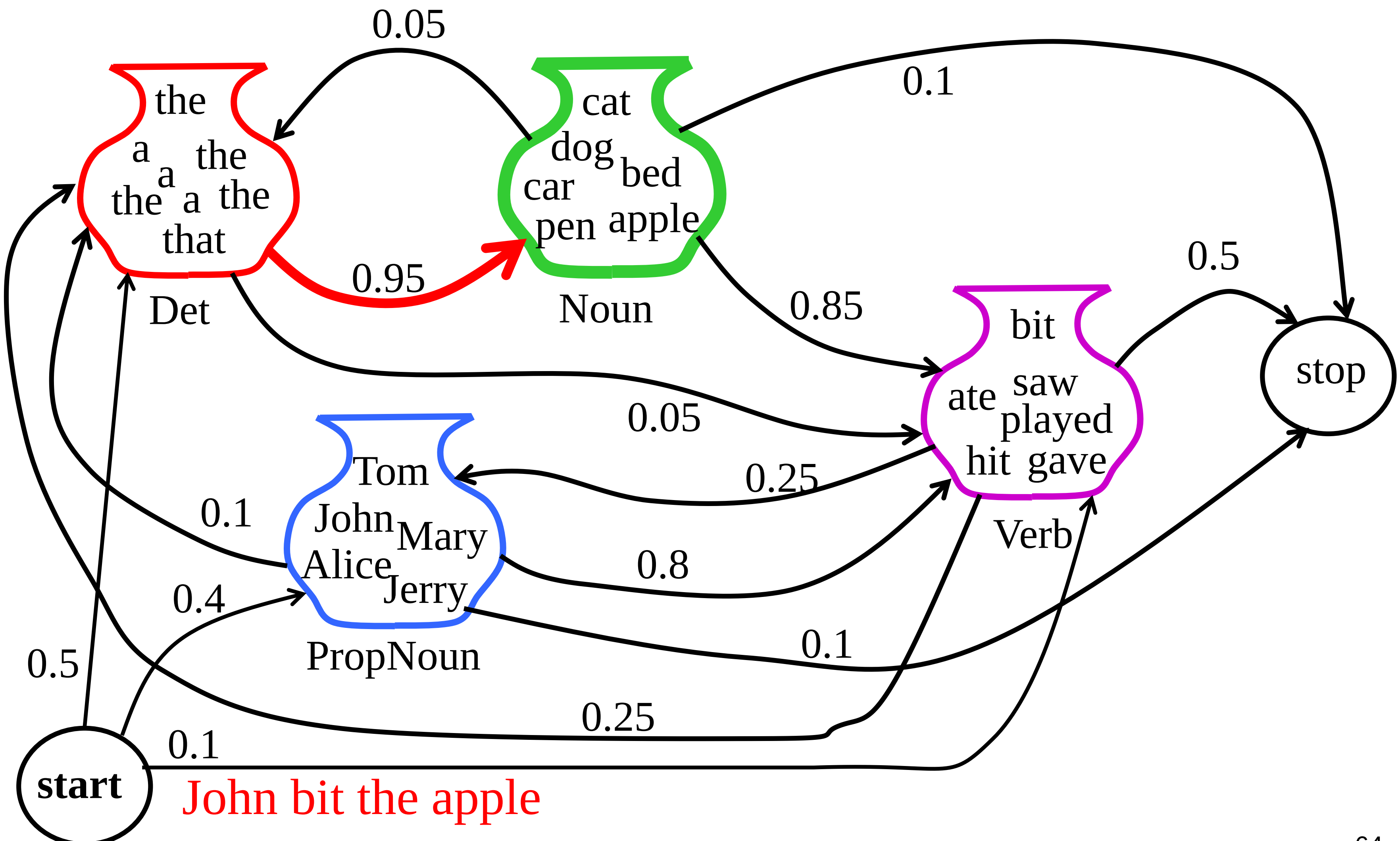
Ray Mooney

Sample HMM Generation



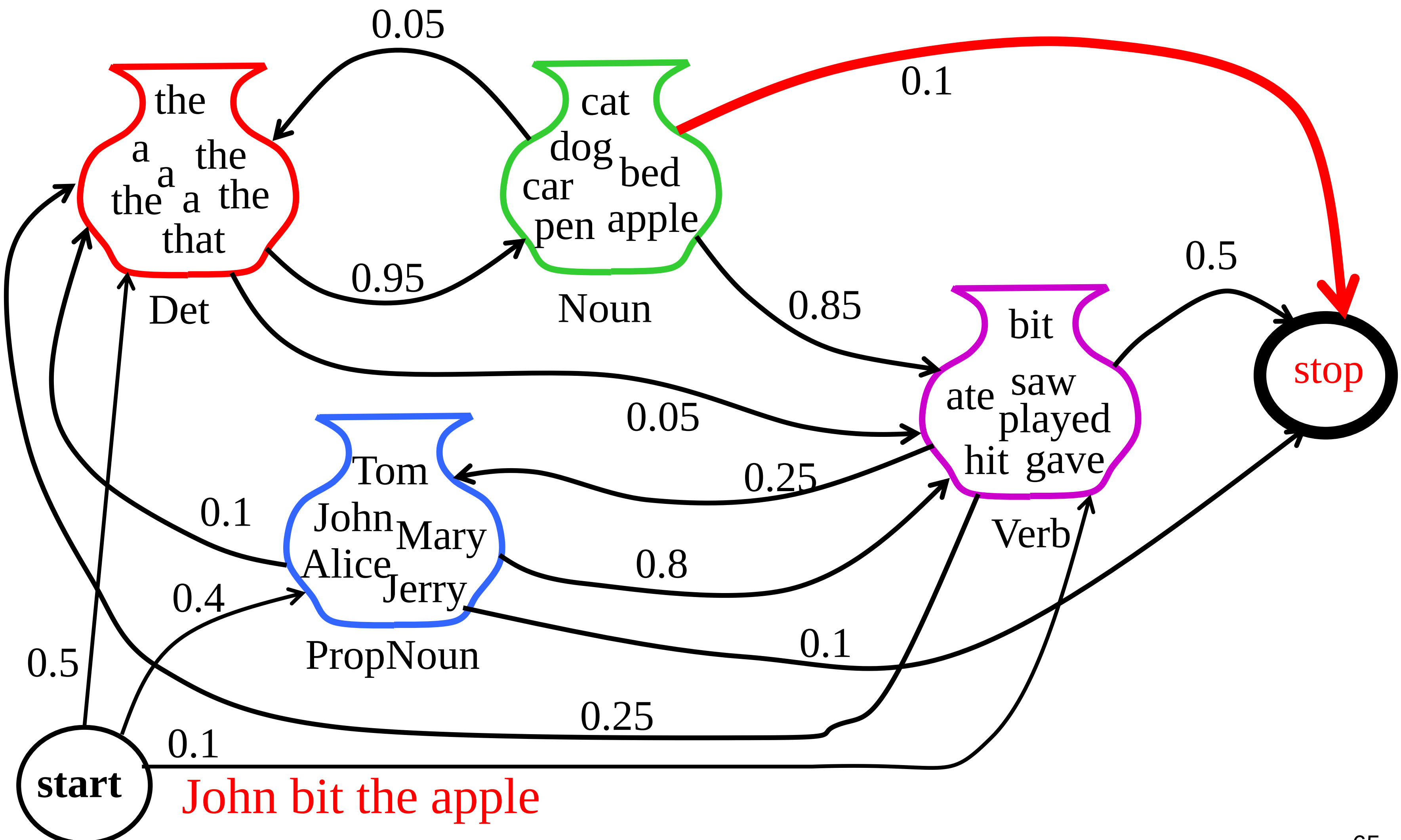
Ray Mooney

Sample HMM Generation



John bit the apple

Sample HMM Generation



Formal Definition of an HMM

- A set of $N+2$ states $S=\{s_0,s_1,s_2, \ldots s_N, s_F\}$
  - Distinguished start state: s_0
  - Distinguished final state: s_F
- A set of M possible observations $V=\{v_1,v_2\ldots v_M\}$
- A state transition probability distribution $A=\{a_{ij}\}$

$$a_{ij} = P(q_{t+1} = s_j \mid q_t = s_i) \qquad 1 \le i, j \le N \text{ and } i = 0, j = F$$

$$\sum_{j=1}^{N} a_{ij} + a_{iF} = 1 \quad 0 \le i \le N$$

- Observation probability distribution for each state j $B=\{b_j(k)\}$

$$b_j(k) = P(v_k \text{ at } t \mid q_t = s_j) \qquad 1 \le j \le N \quad 1 \le \mathrm{k} \le \mathrm{M}$$

- Total parameter set $\lambda=\{A,B\}$

Example

- States = weather (hot/cold)
- Observations = number of ice-creams eaten

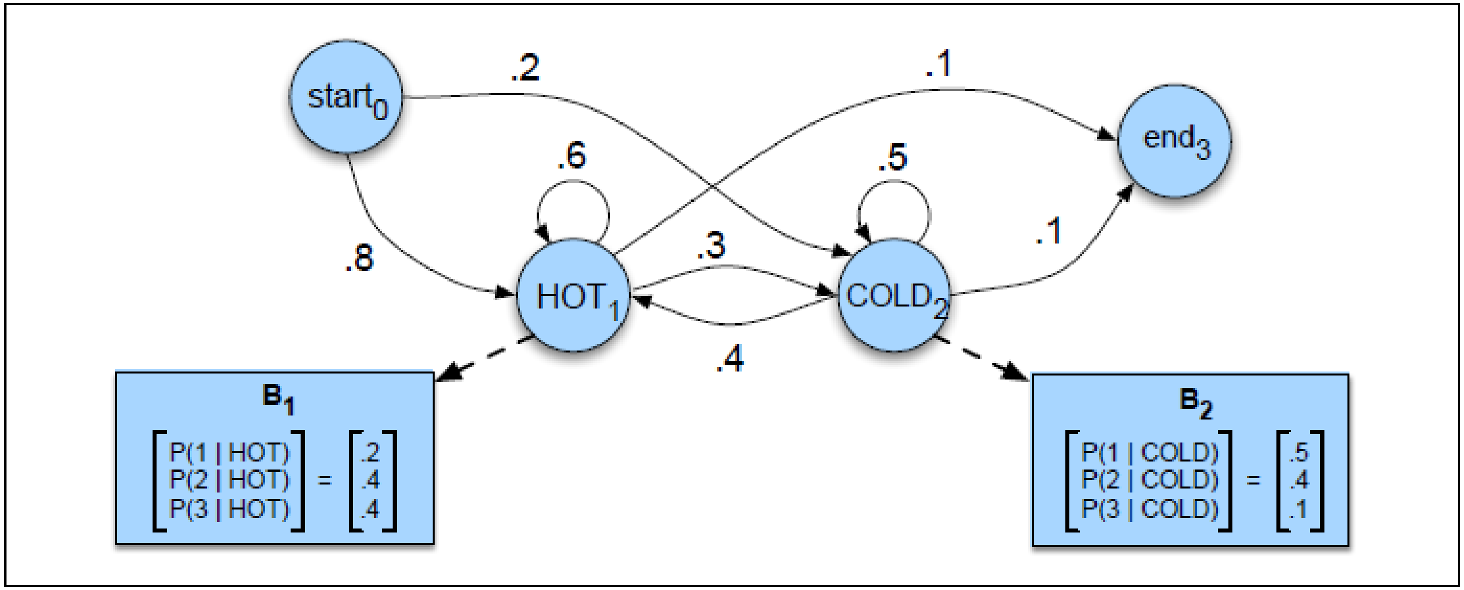


Figure 9.3 A hidden Markov model for relating numbers of ice creams eaten by Jason (the observations) to the weather (H or C, the hidden variables).

Three Useful HMM Tasks

- Compute observation likelihood: How likely is a given sequence of words, regardless of how they might be POS-tagged?
- Estimate most likely *state* sequence: What is the most likely underlying sequence of tags for the observed sequence of words?
- Maximum likelihood training: Estimate transition/emission probabilities given training data (not discussed in this class)

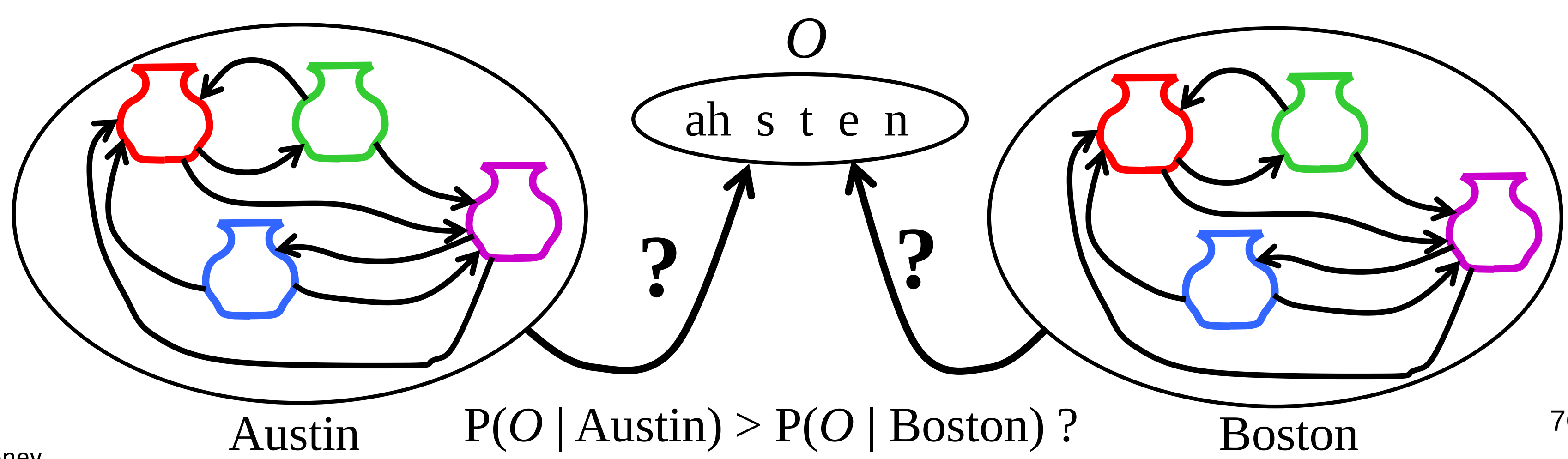
Adapted from Ray Mooney

HMM: Observation Likelihood

- Given a sequence of observations, *O*, and a model with a set of parameters, λ, what is the probability that this observation was generated by this model: $P(O|\lambda)$?
- Allows HMM to be used as a language model: Assigns a probability to each string saying how likely that string is to be generated by the language.
- Example uses:
  - Sequence Classification
  - Most Likely Sequence

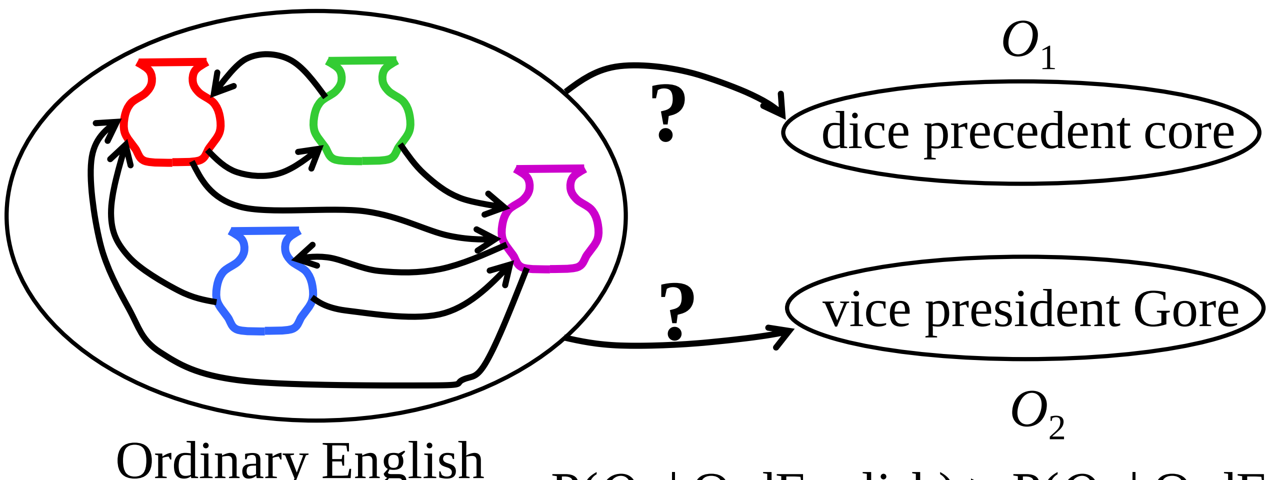
Sequence Classification

- Assume an HMM is available for each category (i.e. language or word).
- What is the most likely category for a given observation sequence, i.e. which category's HMM is most likely to have generated it?
- Used in speech recognition to find most likely word model to have generated a given sound or phoneme sequence.



Most Likely Sequence

- Of two or more possible sequences, which one was most likely generated by a given model?
- Used to score alternative word sequence interpretations in speech recognition.



$P(O_2 \mid \text{OrdEnglish}) > P(O_1 \mid \text{OrdEnglish})$?

HMM: Observation Likelihood Naïve Solution

- Consider all possible state sequences, Q, of length T that the model could have traversed in generating the given observation sequence.
- Compute
  - the probability of a given state sequence from A, and
  - multiply it by the probabilities (from B) of generating each of the given observations in each of the corresponding states in this sequence,
  - to get $P(O,Q| \lambda) = P(O| Q, \lambda) P(Q| \lambda)$.
- Sum this over all possible state sequences to get $P(O| \lambda)$.
- Computationally complex: $O(TN^T)$.

Example

- States = weather (hot/cold), observations = number of ice-creams eaten
- What is the probability of observing {3, 1, 3}?

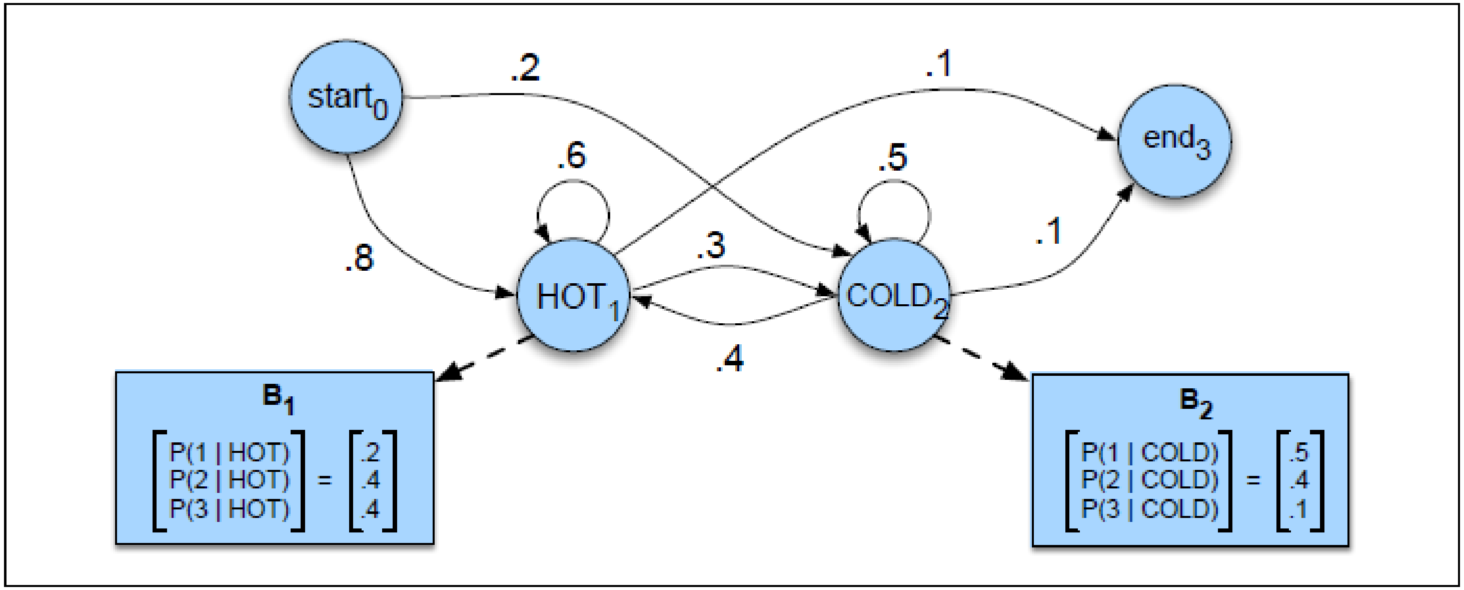


Figure 9.3 A hidden Markov model for relating numbers of ice creams eaten by Jason (the observations) to the weather (H or C, the hidden variables).

Example

- What is the probability of observing {3, 1, 3} *and the state sequence being {hot, hot, cold}?*

$$P(O,Q) = P(O|Q) \times P(Q) = \prod_{i=1}^{T} P(o_i|q_i) \times \prod_{i=1}^{T} P(q_i|q_{i-1})$$

$$P(3\ 1\ 3, \text{hot hot cold}) = P(\text{hot}|\text{start}) \times P(\text{hot}|\text{hot}) \times P(\text{cold}|\text{hot}) \times P(3|\text{hot}) \times P(1|\text{hot}) \times P(3|\text{cold})$$

- What is the probability of observing {3, 1, 3}?

$$P(O) = \sum_{Q} P(O,Q) = \sum_{Q} P(O|Q)P(Q)$$

$$P(3\ 1\ 3) = P(3\ 1\ 3, \text{cold cold cold}) + P(3\ 1\ 3, \text{cold cold hot}) + \ldots$$

HMM: Observation Likelihood Efficient Solution

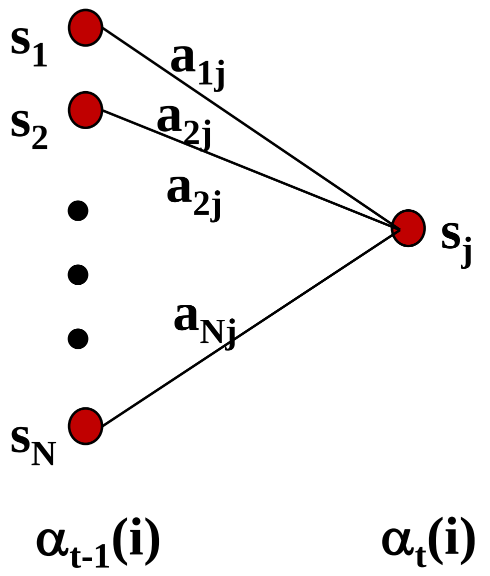
- Due to the Markov assumption, the probability of being in any state at any given time *t* only relies on the probability of being in each of the possible states at time $t-1$.
- Forward Algorithm: Uses dynamic programming to exploit this fact to efficiently compute observation likelihood in $O(TN^2)$ time.
  - Compute a ***forward trellis*** that compactly and implicitly encodes information about all possible state paths.

Forward Probabilities

- Let $\alpha_t(j)$ be the probability of being in state j after seeing the first t observations (by summing over all initial paths leading to j).

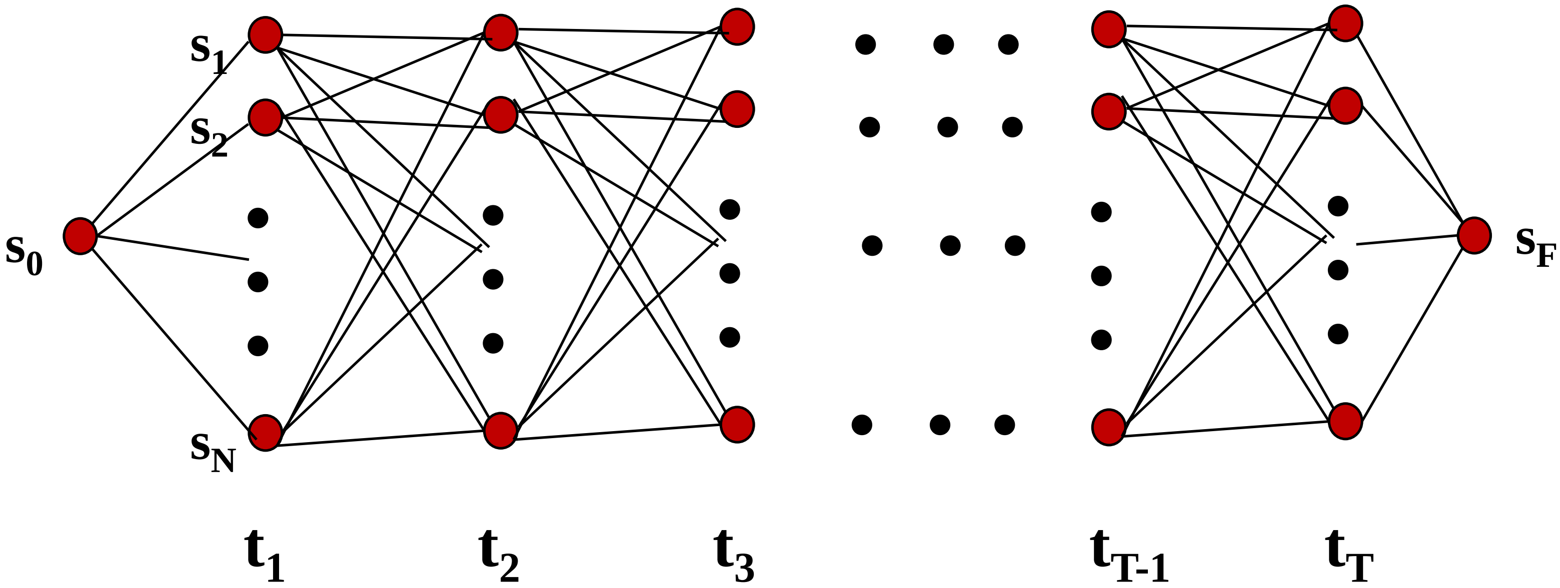
$$\alpha_t(j) = P(o_1, o_2, \ldots o_t,\ q_t = s_j \mid \lambda)$$

Forward Step



- Consider all possible ways of getting to s_j at time t by coming from all possible states s_i and determine probability of each.
- Sum these to get the total probability of being in state s_j at time t while accounting for the first $t-1$ observations.
- Then multiply by the probability of actually observing o_t in s_j.

Forward Trellis



- Continue forward in time until reaching final time point, and sum probability of ending in final state.

Computing the Forward Probabilities

- Initialization

$$\alpha_1(j) = a_{0j} b_j(o_1) \quad 1 \le j \le N$$

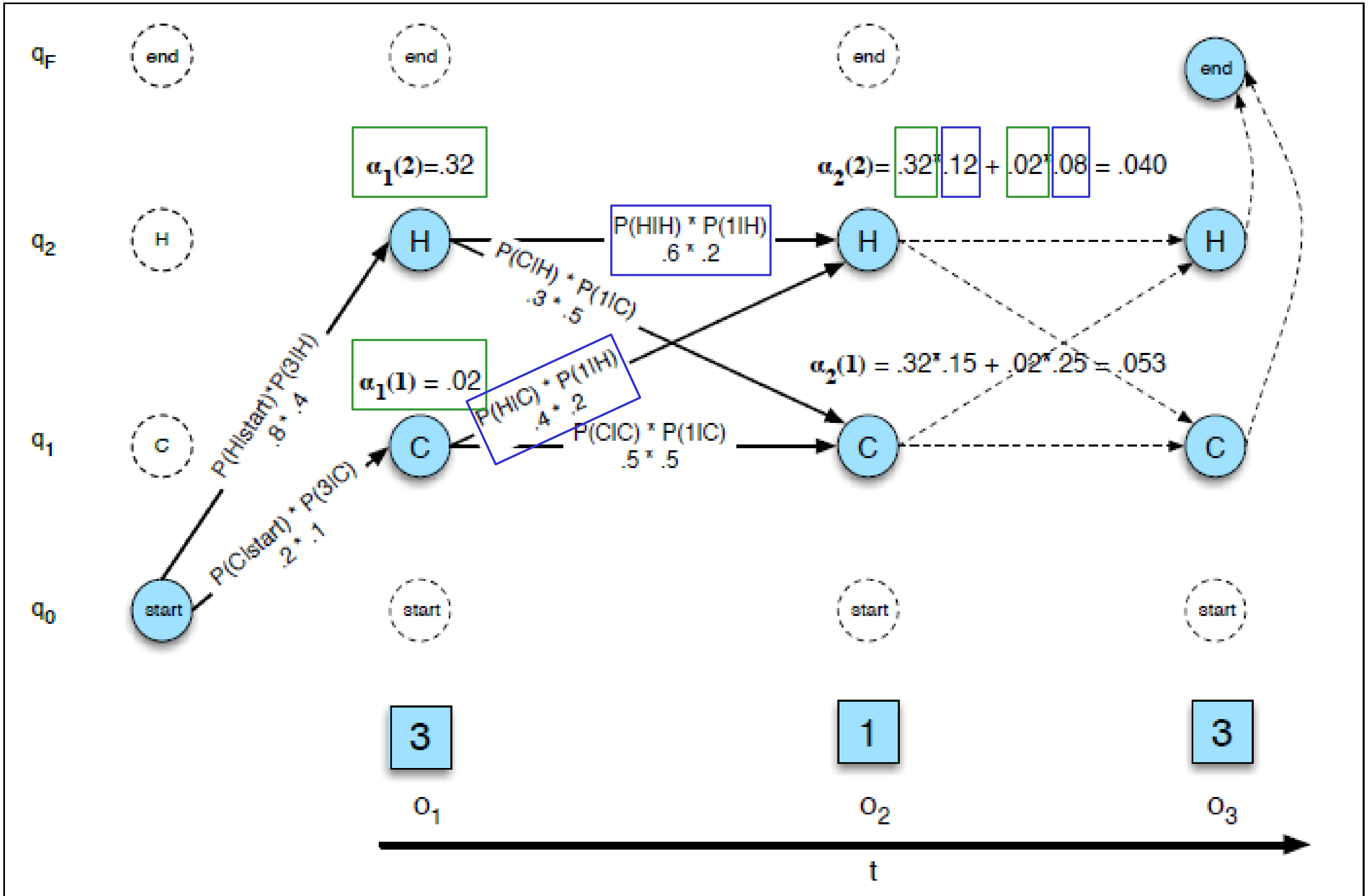
- Recursion

$$\alpha_t(j) = \left[\sum_{i=1}^{N} \alpha_{t-1}(i) a_{ij} \right] b_j(o_t) \quad 1 \le j \le N, \;\; 1 < t \le T$$

- Termination

$$P(O \mid \lambda) = \alpha_{T+1}(s_F) = \sum_{i=1}^{N} \alpha_T(i) a_{iF}$$

Example $\alpha_t(j) = \left[\sum_{i=1}^{N} \alpha_{t-1}(i) a_{ij} \right] b_j(o_t)$



Forward Computational Complexity

- Requires only $O(TN^2)$ time to compute the probability of an observed sequence given a model.
- Exploits the fact that all state sequences must merge into one of the N possible states at any point in time and the Markov assumption that only the last state effects the next one.

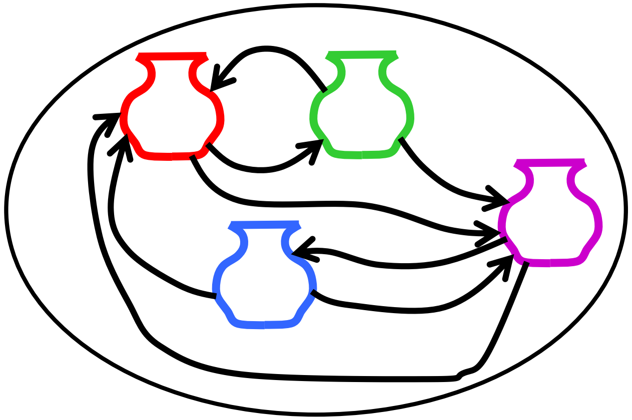
Three Useful HMM Tasks

- Compute observation likelihood: How likely is a given sequence of words, regardless of how they might be POS-tagged?
- Estimate most likely *state* sequence: What is the most likely underlying sequence of tags for the observed sequence of words?
- Maximum likelihood training: Estimate transition/emission probabilities given training data (not discussed in this class)

Adapted from Ray Mooney

Most Likely State Sequence (Decoding)

- Given an observation sequence, O, and a model, λ, what is the most likely state sequence, $Q=q_1,q_2,\ldots q_T$, that generated this sequence from this model?

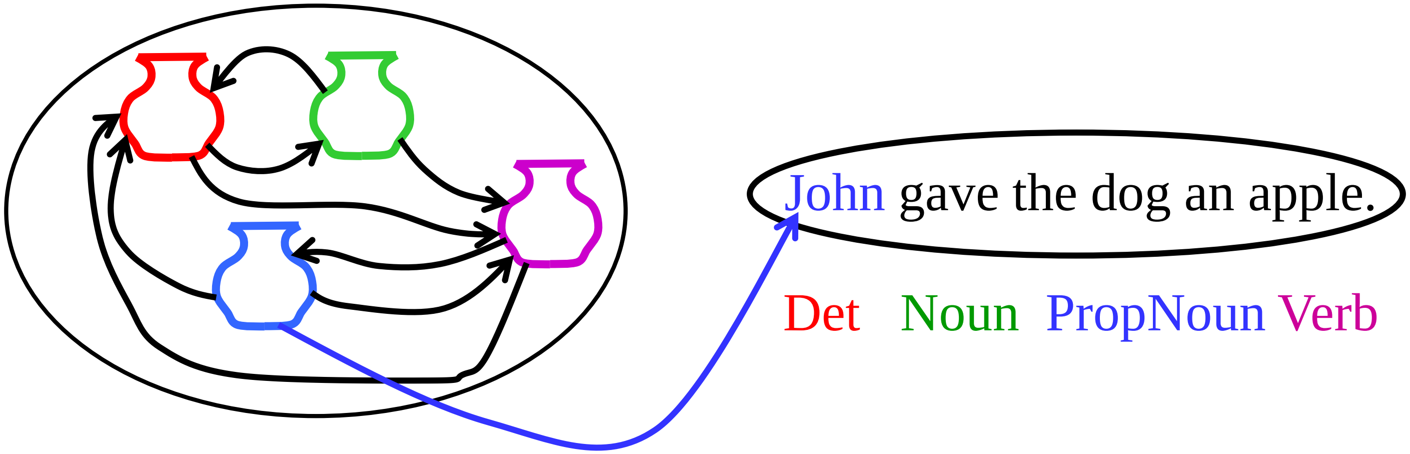


John gave the dog an apple.

Ray Mooney

Most Likely State Sequence

- Given an observation sequence, *O*, and a model, λ, what is the most likely state sequence, $Q=q_1,q_2,\ldots q_T$, that generated this sequence from this model?



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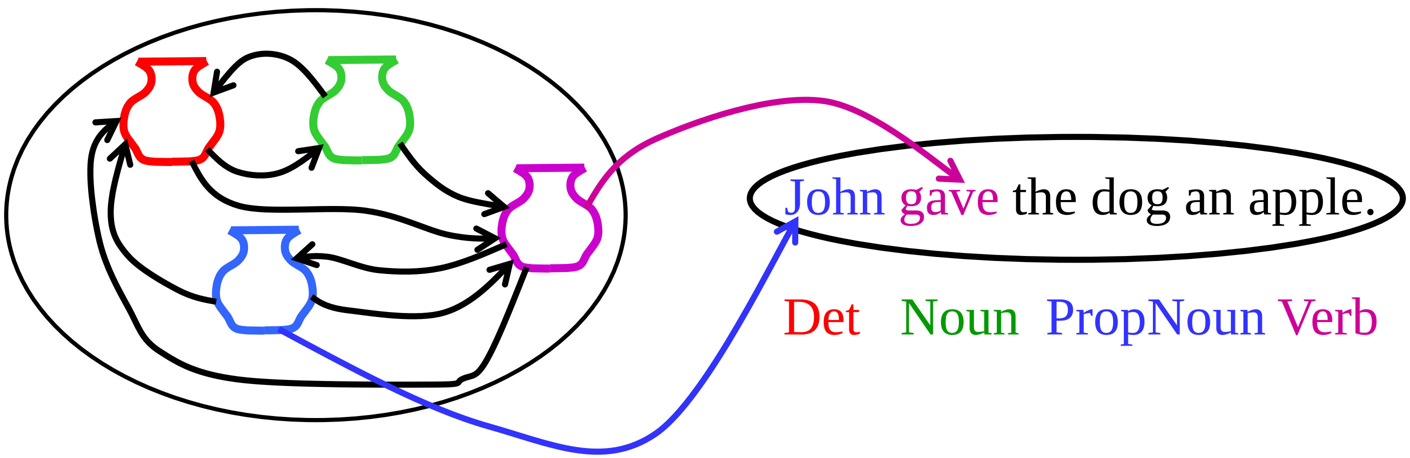

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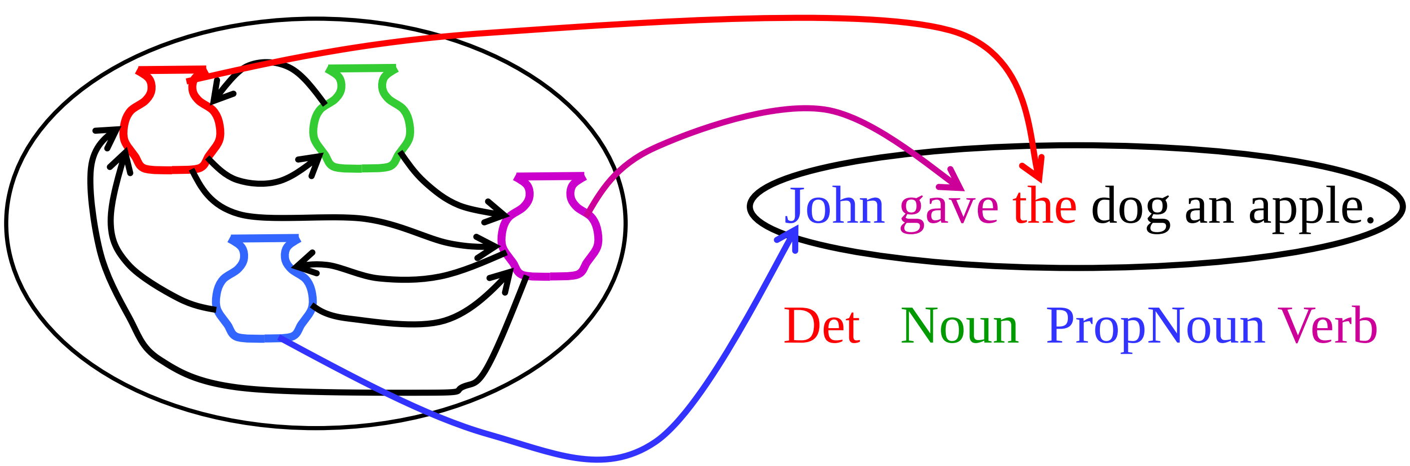

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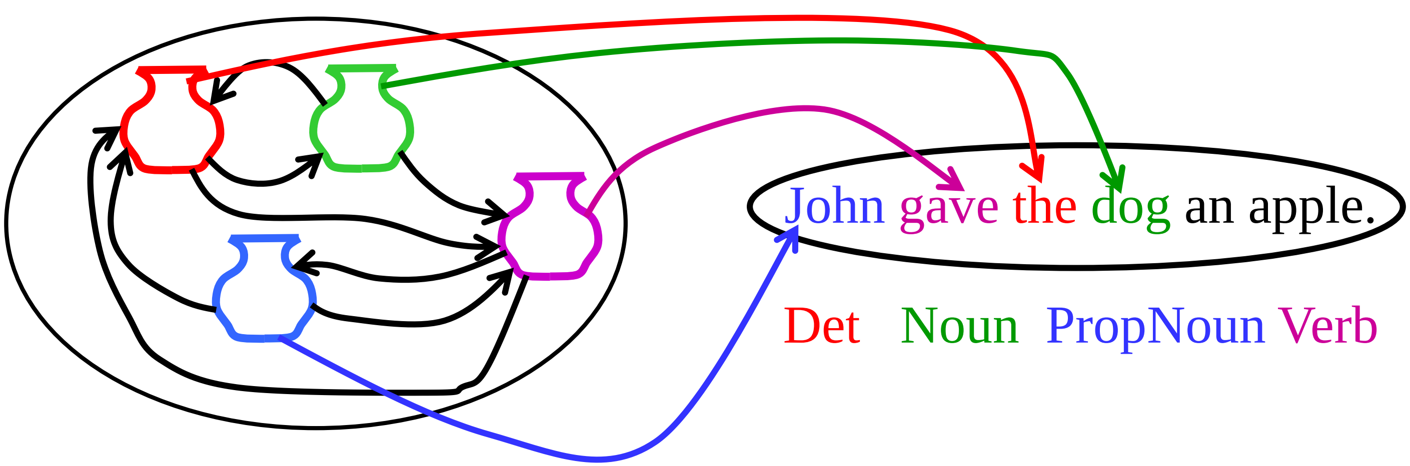

Most Likely State Sequence

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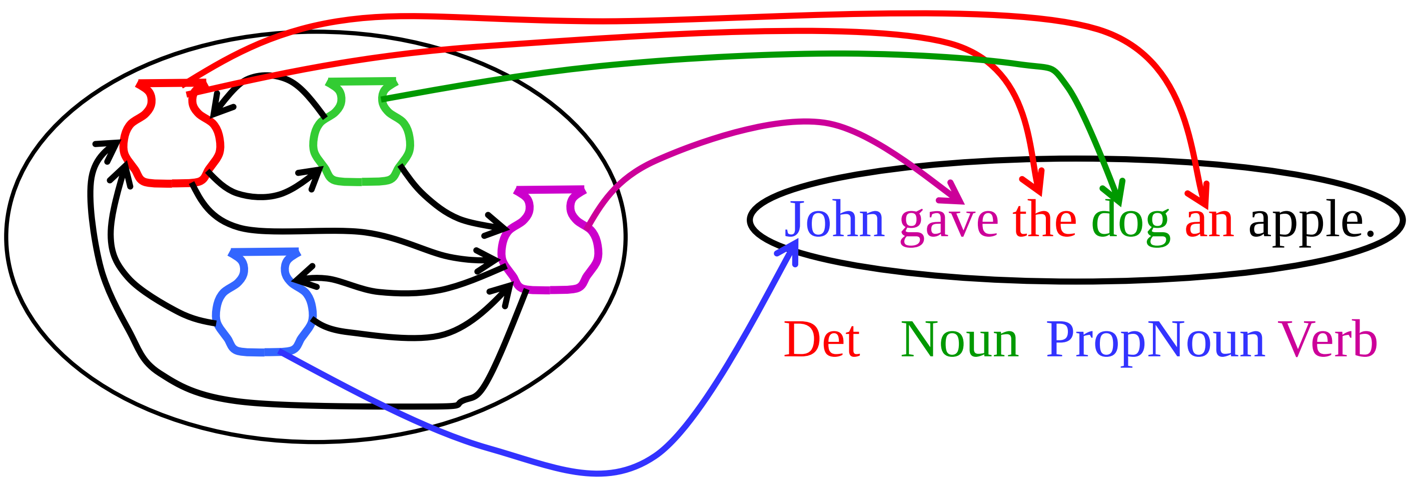
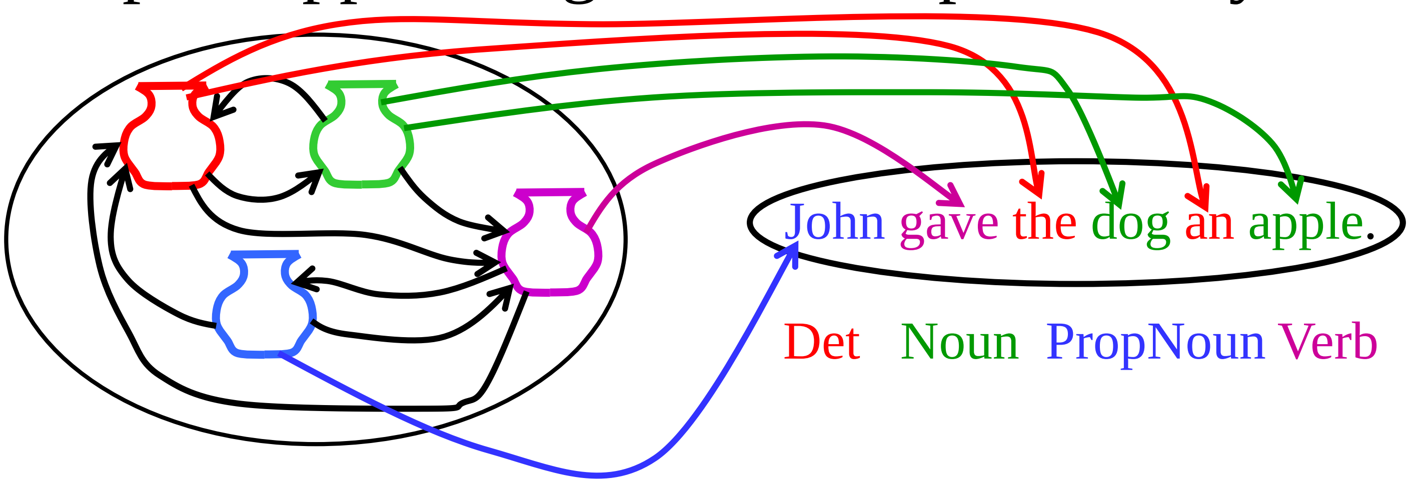


Most Likely State Sequence

- Given an observation sequence, O, and a model, λ, what is the most likely state sequence, $Q=q_1,q_2,\ldots q_T$, that generated this sequence from this model?
- Used for sequence labeling, assuming each state corresponds to a tag, it determines the globally best assignment of tags to all tokens in a sequence using a principled approach grounded in probability theory.



HMM: Most Likely State Sequence Efficient Solution

- Could use naïve algorithm, examining every possible state sequence of length T.
- Dynamic Programming can also be used to exploit the Markov assumption and efficiently determine the most likely state sequence for a given observation and model.
- Standard procedure is called the Viterbi algorithm (Viterbi, 1967) and also has $O(TN^2)$ time complexity.

Viterbi Scores

- Recursively compute the probability of the *most likely* subsequence of states that accounts for the first t observations and ends in state s_j.

$$v_t(j) = \max_{q_0, q_1, \ldots, q_{t-1}} P(q_0, q_1, \ldots, q_{t-1},\ o_1, \ldots, o_t,\ q_t = s_j \mid \lambda)$$

- Also record "backpointers" that subsequently allow backtracing the most probable state sequence.
  - $bt_t(j)$ stores the state at time t-1 that maximizes the probability that system was in state s_j at time t (given the observed sequence).

Computing the Viterbi Scores

- Initialization

$$v_1(j) = a_{0j} b_j(o_1) \quad 1 \le j \le N$$

- Recursion

$$v_t(j) = \max_{i=1}^{N} v_{t-1}(i) a_{ij} b_j(o_t) \quad 1 \le j \le N, \;\; 1 < t \le T$$

- Termination

$$P^* = v_{T+1}(s_F) = \max_{i=1}^{N} v_T(i) a_{iF}$$

Analogous to Forward algorithm except take *max* instead of sum

Computing the Viterbi Backpointers

- Initialization

$$bt_1(j) = s_0 \quad 1 \le j \le N$$

- Recursion

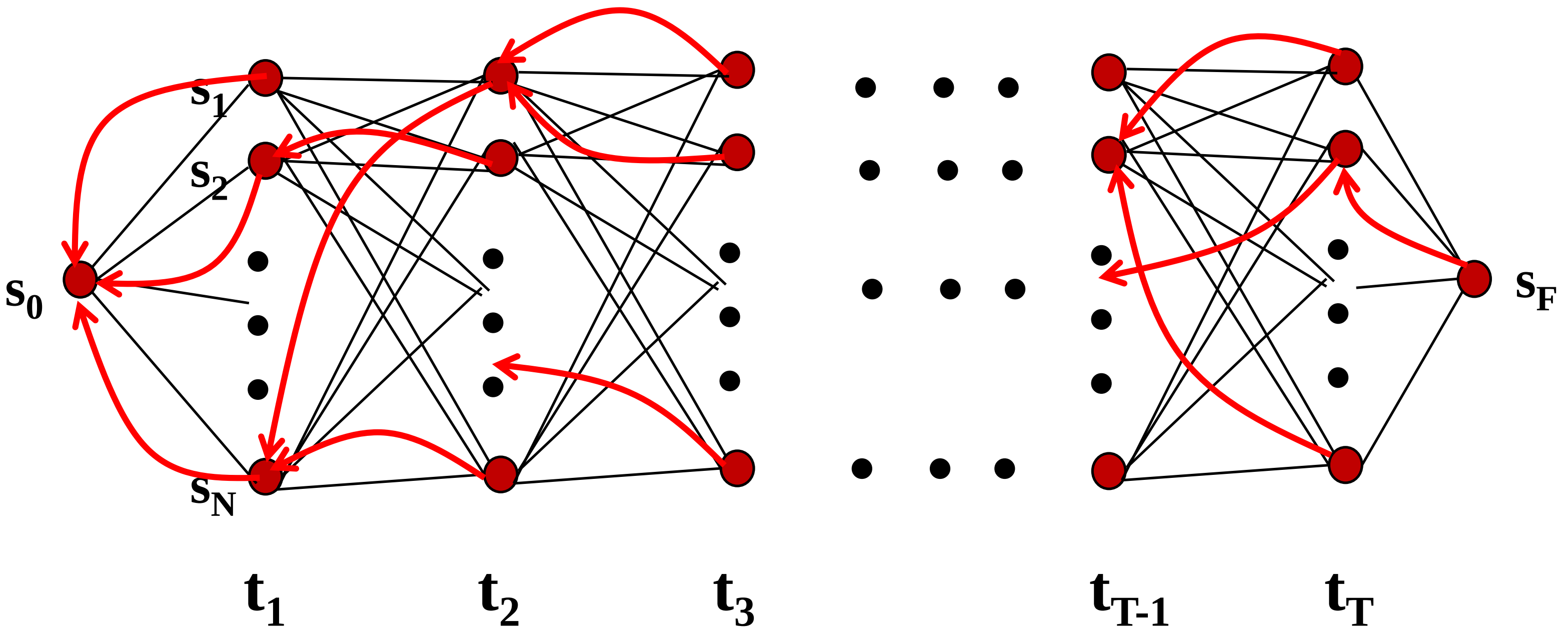
$$bt_t(j) = \underset{i=1}{\overset{N}{\operatorname{argmax}}}\, v_{t-1}(i) a_{ij} b_j(o_t) \quad 1 \le j \le N, \ \ 1 \le t \le T$$

- Termination

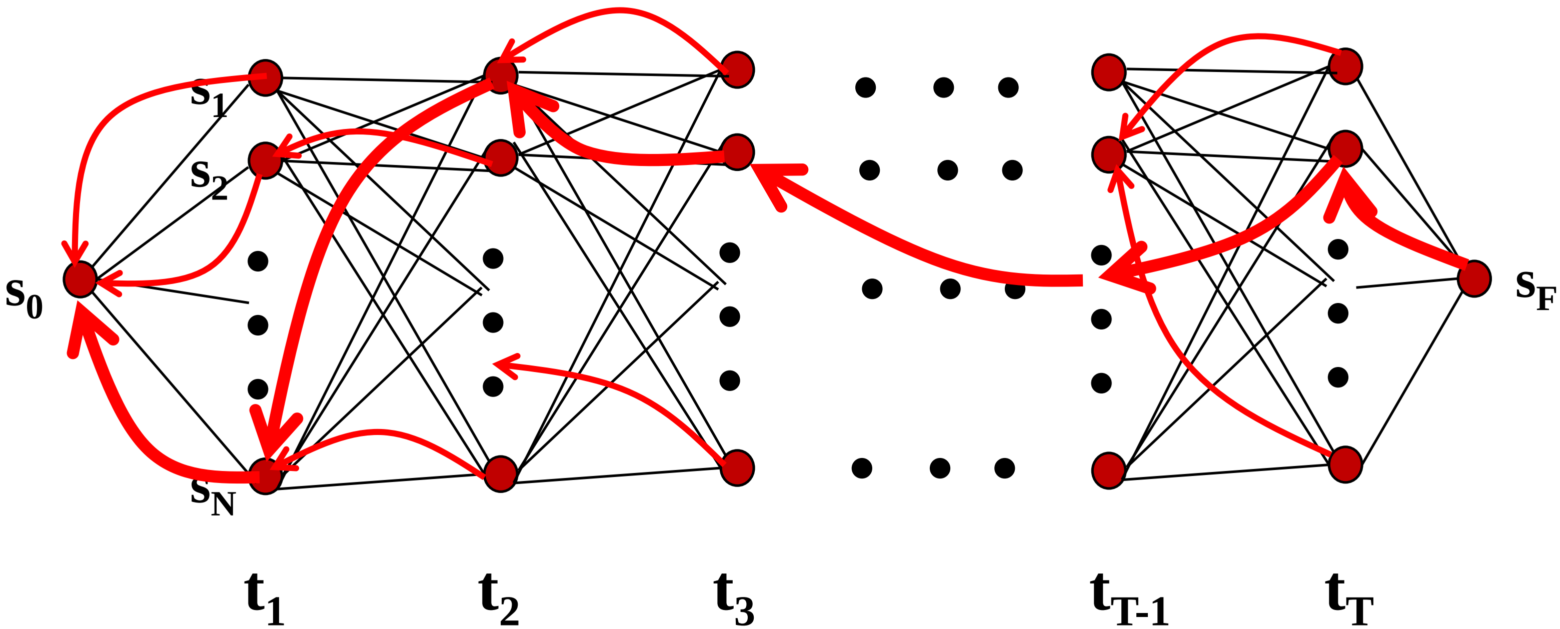
$$q_T{}^* = bt_{T+1}(s_F) = \underset{i=1}{\overset{N}{\operatorname{argmax}}}\, v_T(i) a_{iF}$$

Final state in the most probable state sequence. Follow backpointers to initial state to construct full sequence.

Viterbi Backpointers



Viterbi Backtrace



Most likely Sequence: $s_0\ s_N\ s_1\ s_2\ \ldots s_2\ s_F$

HMM Learning

- **Supervised Learning**: All training sequences are completely labeled (tagged).
- **Unsupervised Learning**: All training sequences are unlabelled (but generally know the number of tags, i.e. states).

Supervised Parameter Estimation

- Estimate state transition probabilities based on tag bigram and unigram statistics in the labeled data.

$$a_{ij} = \frac{C(q_t = s_i, \mathrm{q}_{\mathrm{t+1}} = s_j)}{C(q_t = s_i)}$$

- Estimate the observation probabilities based on tag/word co-occurrence statistics in the labeled data.

$$b_j(k) = \frac{C(q_i = s_j, o_i = v_k)}{C(q_i = s_j)}$$

- Use appropriate smoothing if training data is sparse.

Maximum Likelihood Training

- Given an observation sequence, *O*, what set of parameters, λ, for a given model maximizes the probability that this data was generated from this model ($P(O|\lambda)$)?
- Used to train an HMM model and properly induce its parameters from a set of training data.
- Only need to have an unannotated observation sequence (or set of sequences) generated from the model. Does not need to know the correct state sequence(s) for the observation sequence(s). In this sense, it is unsupervised.

HMM: Maximum Likelihood Training Efficient Solution

- There is no known efficient algorithm for finding the parameters, λ, that truly maximizes $P(O|\lambda)$.
- However, using iterative re-estimation, the Baum-Welch algorithm (a.k.a. forward-backward), a version of a standard statistical procedure called Expectation Maximization (EM), is able to locally maximize $P(O|\lambda)$.
- Recall: K-means (also an example of EM)

Adapted from Ray Mooney

Sketch of Baum-Welch (EM) Algorithm for Training HMMs

Assume an HMM with N states.
Randomly set its parameters $\lambda=(A,B)$
(making sure they represent legal distributions)
Until convergence (i.e. λ no longer changes) do:
E Step: Use the forward/backward procedure to determine the probability of various possible state sequences for generating the training data
M Step: Use these probability estimates to re-estimate values for all of the parameters λ