CPSC 540: Machine Learning Hidden Markov Models

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Last Time: Viterbi Decoding and Message Passing

• Decoding in density models: finding x with highest joint probability:

$$\underset{x_1, x_2, \dots, x_d}{\operatorname{argmax}} p(x_1, x_2, \dots, x_d).$$

• For Markov chains, we find decoding by writing maximization as

$$\max_{x_1, x_2, x_3, x_4} p(x_1, x_2, x_3, x_4) = \max_{x_4} \max_{x_3} p(x_4 \mid x_3) \max_{x_2} p(x_3 \mid x_2) \max_{x_1} p(x_2 \mid x_1) \underbrace{p(x_1)}_{M_1(x_1)}, \underbrace{p(x_1)}_{M_2(x_2)}, \underbrace{p(x_1)}_{M_3(x_3)}, \underbrace{p(x_2)}_{M_3(x_4)}, \underbrace{p(x_1)}_{M_2(x_2)}, \underbrace{p(x_2)}_{M_3(x_3)}, \underbrace{p(x_2)}_{M_3(x_4)}, \underbrace{p(x_2)}_{M$$

• Viterbi decoding computes $M_1(x_1)$ for all x_1 , $M_2(x_2)$ for all x_2 , and so on. The $M_j(x_j)$ functions are called messages (summarize everything about past).

Chapman-Kolmogorov Equations as Message Passing

• We can also view Chapman Kolmogorov equations as message passing:

$$p(x_4) = \sum_{x_3} \sum_{x_2} \sum_{x_1} p(x_1, x_2, x_3, x_4) = \sum_{x_3} \sum_{x_2} \sum_{x_1} p(x_4 \mid x_3) p(x_3 \mid x_2) p(x_2 \mid x_1) p(x_1)$$

$$= \sum_{x_3} p(x_4 \mid x_3) \sum_{x_2} p(x_3 \mid x_2) \sum_{x_1} p(x_2 \mid x_1) M_1(x_1)$$

$$= \sum_{x_3} p(x_4 \mid x_3) \sum_{x_2} p(x_3 \mid x_2) M_2(x_2)$$

$$= \sum_{x_3} p(x_4 \mid x_3) M_3(x_3)$$

$$= M_4(x_4),$$

- Messages $M_i(x_i)$ are the marginals of the Markov chain.
 - So we can view CK equations as Viterbi decoding with "max" replace by "sum".
 - These two methods are also known as "max-product" and "sum-product" algorithms.

Message-Passing Algorithms

- We've discussed several algorithms with similar structure:
 - Viterbi decoding algorithm for decoding in discrete Markov chains.
 - CK equations for marginals in discrete Markov chains.
 - Gaussian updates for marginals in Gaussian Markov chains.
- These are all special cases of message-passing algorithms:
 - **1** Define M_j summarizing all relevant information about the past at time j.
 - ② Use Markov property to write M_j recursively in terms of M_{j-1} .
 - **3** Solve task by computing M_1 , M_2 , ..., M_d .
- "Generalized distributive law" is a framework for describing when/why this works:
 - https://authors.library.caltech.edu/1541/1/AJIieeetit00.pdf
- In some cases we'll also need backwards message V_i ("cost to go"):
 - V_i summarizes all relevant information about the future at time j.

Backwards "Cost to Go" Messages

• Using backwards messages $V_i(x_i)$ to (innefficiently) compute $p(x_1)$:

$$\begin{split} p(x_1) &= \sum_{x_2} \sum_{x_3} \sum_{x_4} p(x_1, x_2, x_3, x_4) = \sum_{x_2} \sum_{x_3} \sum_{x_4} p(x_1) p(x_2 \mid x_1) p(x_3 \mid x_2) p(x_4 \mid x_3) \\ &= p(x_1) \sum_{x_2} p(x_2 \mid x_1) \sum_{x_3} p(x_3 \mid x_2) \sum_{x_4} p(x_4 \mid x_3) \\ &= p(x_1) \sum_{x_2} p(x_2 \mid x_1) \sum_{x_3} p(x_3 \mid x_2) \sum_{x_4} p(x_4 \mid x_3) \underbrace{V_4(x_4)}_{=1} \\ &= p(x_1) \sum_{x_2} p(x_2 \mid x_1) \underbrace{\sum_{x_3} p(x_3 \mid x_2)}_{1} \underbrace{V_3(x_3)}_{1} \\ &= p(x_1) \underbrace{\sum_{x_2} p(x_2 \mid x_1) \underbrace{V_2(x_2)}_{1}}_{1} \\ &= p(x_1) \underbrace{V_1(x_1)}_{1}. \end{split}$$

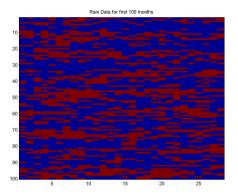
- Observe that backwards messages $V_j(x_j)$ are not probabilities as in CK equations.
 - But they summarize everything you need to know about the future.
 - Can use this structure to condition on the future, and compute things like $p(x_1 \mid x_4)$.

Forward-Backward Algorithm

- Computing all $M_i(x_i)$ and $V_i(x_i)$ is called the forward-backward algorithm.
 - Not interesting for Markov chains since $V_j(x_j) = 1$ for all j and x_j .
- Why do we need both types of messages?
 - Can efficiently compute all conditionals $p(x_j = s \mid x_{10} = 3)$ (for all j and s).
 - Messages are modified when you condition (see bonus slides).
 - The modified $V_i(x_i)$ will reflect "what you need to know about the future events".
 - Can be used to compute probabilities in generalizations of Markov chains (next).
 - In this setting the forward messages may not be probabilities either.
 - In reinforcement learning, estimating the "cost to go" ("value") function is the goal.
 - We aren't covering RL, but understanding Markov chains will help you understand RL.

Back to the Rain Data

• We previously considered the "Vancouver Rain" data:



- We said that a homogeneous Markov chain is a good model:
 - Captures direct dependency between adjcaent days.

Back to the Rain Data

- But doesn't it rain less in the summer?
- There are hidden clusters in the data not captured by the Markov chain.
 - But mixture of independent models are inefficient at representing direct dependency.
- Mixture of Markov chains could capture direct dependence and clusters,

$$p(x_1, x_2, \dots, x_d) = \sum_{c=1}^k p(z=c) \underbrace{p(x_1 \mid z=c) p(x_2 \mid x_1, z=c) \cdots p(x_d \mid x_{d-1}, z=c)}_{\text{Markov chain } c}.$$

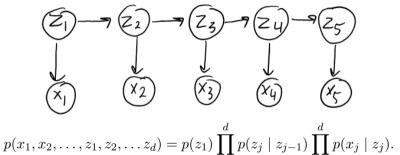
- Cluster z chooses which homogeneous Markov chain parameters to use.
 - We could learn that we're more likely to have rain in winter.
 - Can modify CK equations to take into account z, and then apply EM.

Back to the Rain Data

- The rain data is artificially divideded into months.
- We previously discussed viewing rain data as one very long sequence (n = 1).
- We could apply homogeneous Markov chains due to parameter tieing.
- But a mixture doesn't make sense when n=1.
- What we want: different "parts" of the sequence come from different clusters.
 - We transition from "summer" cluster to "fall" cluster at some time j.
- One way to address this ("hidden" Markov model):
 - Let each day have it's own cluster.
 - Have a Markov dependency between cluster values of adjacent days.

Hidden Markov Models

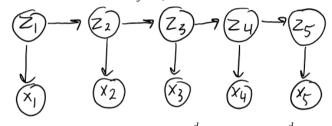
• Hidden Markov models have each x_i depend on hidden Markov chain.



- We're going to learn clusters z_i and the hidden dynamics.
 - Hidden cluster z_i could be "summer" or "winter" (we're learning the clusters).
 - Transition probability $p(z_j \mid z_{j-1})$ is probability of staying in "summer".
 - Emission probability $p(x_i \mid z_i)$ is probability of "rain" during "summer".

Hidden Markov Models

• Hidden Markov models have each x_i depend on hidden Markov chain.

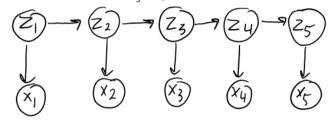


$$p(x_1, x_2, \dots, z_1, z_2, \dots z_d) = p(z_1) \prod_{i=2}^{a} p(z_i \mid z_{j-1}) \prod_{i=1}^{a} p(x_i \mid z_j).$$

- You observe the x_i values but do not see the z_i values.
 - CK equations won't work since $p(z_1 = s)$ depends on future x_i values.
- But forward-backward algorithm can be used to compute probailities.
 - And subsequently learn with EM.

Hidden Markov Models

• Hidden Markov models have each x_i depend on hidden Markov chain.



- Note that the x_i can be continuous even with discrete clusters z_i .
 - You could have a "mixture of Gaussians" with cluster changing in time.
- If the z_i are continuous it's often called a state-space model.
 - If everything is Gaussian, it leads to Kalman filtering.
 - Keywords for non-Gaussian: unscented Kalman filter and particle filter.
- Variants of HMMs are probably the most-used time-series model...

Applications of HMMs and Kalman Filters

Applications [edit]

HMMs can be applied in many fields where the goal is to recover a data sequence that is not immediately observable (but other data that depend on the sequence are).

- . Single Molecule Kinetic analysis^[16]
- Cryptanalysis
- . Speech recognition
- . Speech synthesis
- . Part-of-speech tagging
- . Document Separation in scanning solutions
- . Machine translation
- . Partial discharge
- . Gene prediction
- . Alignment of bio-sequences
- . Time Series Analysis
- . Activity recognition
- . Protein folding^[17]
- . Metamorphic Virus Detection[18]
- . DNA Motif Discovery^[19]

Applications [edit]

- . Attitude and Heading Reference Systems
- . Autopilot
- . Battery state of charge (SoC) estimation^{[39][40]}
- . Brain-computer interface
- . Chaotic signals
- Tracking and Vertex Fitting of charged particles in Particle Detectors^[41]
- . Tracking of objects in computer vision
- . Dynamic positioning

- Economics, in particular macroeconomics, time series analysis, and econometrics^[42]
- series analysis, and econometrics(42)
- . Orbit Determination
- . Power system state estimation
- . Radar tracker
- Satellite navigation systems
- . Seismology^[43]
- . Sensorless control of AC motor variable-frequency drives

- . Simultaneous localization and mapping
- . Speech enhancement
- . Visual odometry
- . Weather forecasting
- . Navigation system
- . 3D modeling
- . Structural health monitoring
- . Human sensorimotor processing^[44]

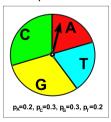
Example: Modeling DNA Sequences

- A nice demo of independent vs. Markov vs. HMMs for DNA sequences:
 - http://a-little-book-of-r-for-bioinformatics.readthedocs.io/en/latest/src/chapter10.html



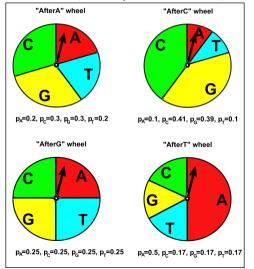
https://www.tes.com/lessons/WE5E9RncBhieAQ/dna

• Independent model for elements of sequence:



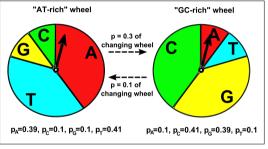
Example: Modeling DNA Sequences

• Markov model for elements of sequence (dependence on previous symbol):



Example: Modeling DNA Sequences

• Hidden Markov model (HMM) for elements of sequence (two hidden clusters):



- Can reflect that probabilities are different in different regions.
 - The actual regions are not given, but instead are nuissance variables handled by EM.
- You probably get a better model by consider hidden Markov and visible Markov.
 - With 2 hidden clusters, you would have 8 "probability wheels" (4 per cluster).
 - Would have "treewidth 2", which we'll show later means it's tractable to use.

Who is Guarding Who?

- There is a lot of data on offense of NBA basketball players.
 - Every point and assist is recorded, more scoring gives more wins and \$\$\$.
- But how do we measure defense?
 - We need to know who each player is guarding.

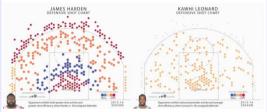


Figure 2a. Graphical depiction of a defender's volume (size) and disruption scores (color). Kawhi Leonard tends to suppress shots on the perimeter. More comparisons are provided in the Appendix.

http://www.lukebornn.com/papers/franks_ssac_2015.pdf

- HMMs can be used to model who is guarding who over time.
 - https://www.youtube.com/watch?v=JvNkZdZJBt4

Outline

- Hidden Markov Models
- 2 Directed Acyclic Graphical Models

Higher-Order Markov Models

Markov models use a density of the form

$$p(x) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2)p(x_4 \mid x_3) \cdots p(x_d \mid x_{d-1}).$$

- They support efficient computation but Markov assumption is strong.
- A more flexible model would be a second-order Markov model,

$$p(x) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2, x_1)p(x_4 \mid x_3, x_2) \cdots p(x_d \mid x_{d-1}, x_{d-2}),$$

or even a higher-order models.

- General case is called directed acyclic graphical (DAG) models:
 - They allow dependence on any subset of previous features.

DAG Models

• As in Markov chains, DAG models use the chain rule to write

$$p(x_1, x_2, \dots, x_d) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2) \cdots p(x_d \mid x_1, x_2, \dots, x_{d-1}).$$

• We can alternately write this as:

$$p(x_1, x_2, \dots, x_d) = \prod_{j=1}^d p(x_j \mid x_{1:j-1}).$$

- In Markov chains, we assumed x_i only depends on previous x_{i-1} given past.
- In DAGs, x_j can depend on any subset of the past $x_1, x_2, \ldots, x_{j-1}$.

DAG Models

• We often write joint probability in DAG models as

$$p(x_1, x_2, \dots, x_d) = \prod_{j=1}^d p(x_j \mid x_{\mathsf{pa}(j)}),$$

where pa(j) are the "parents" of node j.

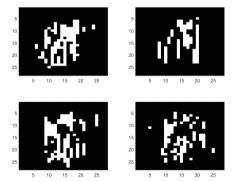
- For Markov chains the only "parent" of j is (j-1).
- ullet If we have k parents we only need 2^{k+1} parameters.
- This corresponds to a set of conditional independence assumptions,

$$p(x_j \mid x_{1:j-1}) = p(x_j \mid x_{pa(j)}),$$

that we're independent of previous non-parents given the parents.

MNIST Digits with Markov Chains

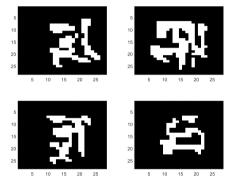
• Recall trying to model digits using an inhomogeneous Markov chain:



Only models dependence on pixel above, not on 2 pixels above nor across columns.

MNIST Digits with DAG Model (Sparse Parents)

• Samples from a DAG model with 8 parents per feature:



Parents of (i, j) are 8 other pixels in the neighbourhood ("up by 2, left by 2"):

$$\{(i-2,j-2),(i-1,j-2),(i,j-2),(i-2,j-1),(i-1,j-1),(i,j-1),(i-2,j),(i-1,j)\}.$$

From Probability Factorizations to Graphs

- DAG models are also known as "Bayesian networks" and "belief networks".
- "Graphical" name comes from visualizing parents/features as a graph:
 - We have a node for each feature j.
 - We place an edge into j from each of its parents.
- The DAG representation for a Markov chains is:



- Different than "state transition diagrams": edges are between variables (not states).
- This graph is not just a visualization tool:
 - Can be used to test arbitrary conditional independences ("d-separation").
 - Graph structure tells us whether message passing is efficient ("treewidth").

With product of independent we have

$$p(x) = \prod_{j=1}^{d} p(x_j),$$

so $pa(i) = \emptyset$ and the graph is:







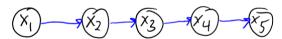




With Markov chain we have

$$p(x) = p(x_1) \prod_{j=2}^{d} p(x_j \mid x_{j-1}),$$

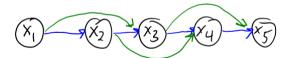
so $pa(j) = \{j-1\}$ and the graph is:



With second-order Markov chain we have

$$p(x) = p(x_1)p(x_2 \mid x_1) \prod_{j=3}^{d} p(x_j \mid x_{j-1}, x_{j-2}),$$

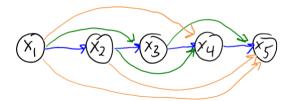
so $pa(j) = \{j-2, j-1\}$ and the graph is:



With general distribution we have

$$p(x) = \prod_{j=1}^{d} p(x_j \mid x_{1:j-1}).$$

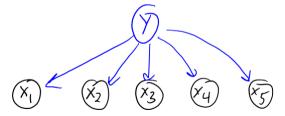
so $pa(j) = \{1, 2, \dots, j-1\}$ and the graph is:



In naive Bayes (or GDA with diagonal Σ) we add an extra variable y and use

$$p(y,x) = p(y) \prod_{j=1}^{d} p(x_j | y),$$

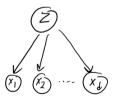
which has $pa(y) = \emptyset$ and $pa(x_j) = y$ giving



With mixture of independent models we have

$$p(z,x) = p(z) \prod_{j=1}^{d} p(x_j \mid z).$$

which has $pa(z) = \emptyset$ and $pa(x_i) = z$ giving same structure as naive Bayes:

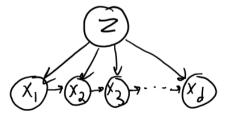


Since structure is the same, many computations will be similar.

With mixture of Markov chains models we have

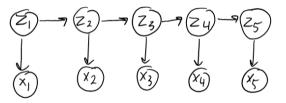
$$p(x_1, x_2, \dots, x_d, z) = p(z)p(x_1 \mid z) \prod_{i=2}^d p(x_j \mid x_{j-1}, z).$$

which has $pa(z) = \emptyset$ and $pa(x_j) = \{x_{j-1}, z\}$:



Sometimes it's easier to present a model using the graph.

In hidden Markov models we have this structure:



The graph and variable names already give you an idea of what this model does:

- We have hidden variables z_i that follow a Markov chain.
- Each feature x_i depends on corresponding hidden variable z_i .

• Instead of factorizing by variables *j*, could factor into blocks *b*:

$$p(x) = \prod_b p(x_b \mid x_{\mathsf{pa}(b)}),$$

and have the nodes be blocks (usually assuming full connectivity within the block).

• With mixture of Gaussian and full covariances we have

$$p(z,x) = p(z)p(x \mid z).$$

• The corresponding graph structure is:

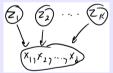


• Gaussian generative classifiers (GDA) have the same structure.

With probabilistic PCA we have

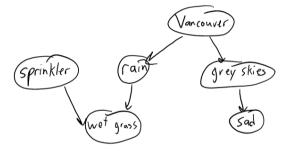
$$p(z,x) = p(x \mid z) \prod_{c=1}^{k} p(z_c).$$

The corresponding graph structure is:



The data x comes from a set of independent parents (latent factors).

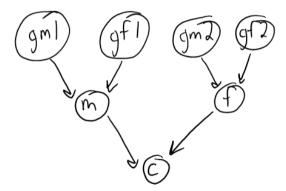
We can consider less-structured examples,



The corresponding factorization is:

$$p(S, V, R, W, G, D) = p(S)p(V)p(R \mid V)p(W \mid S, R)p(G \mid V)p(D \mid G).$$

We can consider phylogeny (family trees):



Summary

- Message-passing allow efficient calculations with Markov chains.
- Hidden Markov models model time-series with hidden per-time cluster.
 - Tons of applications, typically more realistic than Markov models.
- DAG models factorize joint distribution into product of conditionals.
 - Assume conditionals depend on small number of "parents".
 - Joint distribution of models we've discussed can be written as DAG models.
- Next time: the IID assumption as a graphical model?

Computing Conditional Probabilities

- Previously: Monte Carlo for approximating conditional probabilities
- For Gaussian/discrete Markov chains, we can do better than rejection sampling.
 - We can generate exact samples from conditional distribution (bonus slide).
 - Rejection sampling is not needed, relies on "backwards sampling" in time.
 - **2** We can find conditional decoding $\max_{x \mid x_{i'} = c} p(x)$:
 - Run Viterbi decoding with $M_{j'}(c) = 1$ and $M_{j'}(c') = 0$ for $c \neq c'$.
 - **3** We can find univariate conditionals, $p(x_j \mid x_{j'})$.
- Example of computing $p(x_1 = c \mid x_3 = 1)$ in a length-4 discrete Markov chain:

$$p(x_1 = c \mid x_3 = 1) \propto p(x_1 = c, x_3 = 1)$$

$$= \sum_{x_4} \sum_{x_2} p(x_1 = c, x_2, x_3 = 1, x_4),$$

where the normalizing constant is the marginal $p(x_3 = 1)$.

• This is a sum over k^{d-2} possible assignments to other variables.

Distributing Sum across Product

• Fortunately, the Markov property makes the sums simplify as before:

$$\sum_{x_4} \sum_{x_2} p(x_1 = c, x_2, x_3 = 1, x_4) = \sum_{x_4} \sum_{x_3 = 1} \sum_{x_2} \sum_{x_1 = c} p(x_4 \mid x_3) p(x_3 \mid x_2) p(x_2 \mid x_1) p(x_1)$$

$$= \sum_{x_4} \sum_{x_3 = 1} \sum_{x_2} p(x_4 \mid x_3) p(x_3 \mid x_2) \sum_{x_1 = c} p(x_2 \mid x_1) p(x_1)$$

$$= \sum_{x_4} \sum_{x_3 = 1} p(x_4 \mid x_3) \sum_{x_2} p(x_3 \mid x_2) \sum_{x_1 = c} p(x_2 \mid x_1) M_1(x_1)$$

$$= \sum_{x_4} \sum_{x_3 = 1} p(x_4 \mid x_3) \sum_{x_2} p(x_3 \mid x_2) M_2(x_2)$$

$$= \sum_{x_4} \sum_{x_3 = 1} p(x_4 \mid x_3) M_3(x_3)$$

$$= \sum_{x_4} M_4(x_4),$$

where $M_i(x_i)$ now sums over paths ending in x_i instead of maximizing.

• And we set $M_1(c') = 0$ if $c' \neq c$ and $M_3(c') = 0$ for $c' \neq 1$.

Conditionals via Backwards Messages

Performing our conditional calculation using backwards messages.

$$\begin{split} \sum_{x_4} \sum_{x_2} p(x_1 = c, x_2, x_3 = 1, x_4) &= \sum_{x_1 = c} \sum_{x_2} \sum_{x_3 = 1} \sum_{x_4} p(x_4 \mid x_3) p(x_3 \mid x_2) p(x_2 \mid x_1) p(x_1) \\ &= \sum_{x_1 = c} p(x_1) \sum_{x_2} p(x_2 \mid x_1) \sum_{x_3 = 1} p(x_3 \mid x_2) \sum_{x_4} p(x_4 \mid x_3) \\ &= \sum_{x_1 = c} p(x_1) \sum_{x_2} p(x_2 \mid x_1) \sum_{x_3 = 1} p(x_3 \mid x_2) \sum_{x_4} p(x_4 \mid x_3) \underbrace{V_4(x_4)}_{=1} \\ &= \sum_{x_1 = c} p(x_1) \sum_{x_2} p(x_2 \mid x_1) \sum_{x_3 = 1} p(x_3 \mid x_2) V_3(x_3) \\ &= \sum_{x_1 = c} p(x_1) \sum_{x_2} p(x_2 \mid x_1) V_2(x_2) \\ &= \sum_{x_1 = c} p(x_1) V_1(x_1). \end{split}$$

Forward-Backward Algorithm

• Generic forward and backward messages for discrete marginals have the form

$$M_j(x_j) = \sum_{x_{j-1}} p(x_j \mid x_{j-1}) M_{j-1}(x_{j-1}), \quad V_j(x_j) = \sum_{x_{j+1}} p(x_{j+1} \mid x_j) V_{j+1}(x_{j+1}).$$

- We can compute $p(x_i = c \mid x_{i'} = c')$ using only forward messages:
 - Set $M_i(c) = 1$ and $M_{i'}(c') = 1$.
- Why we would need backward messages?

Forward-Backward Algorithm

- We can compute $p(x_j = c \mid x_{j'} = c')$ for all j in $O(dk^2)$ with both messages.
- ullet First compute all message normally with $M_{j'}(c')=1$ and $V_{j'}(c')=1$. (Other $M_{j'}$ and $V_{j'}$ are set to 0)
- We then have that
 - $M_j(x_j)$ sums up all the paths that end in state x_j (with $x_{j'}=c'$).
 - $V_i(x_i)$ sums up all the paths that start in state x_i (with $x_{i'} = c'$).
 - We can combine these values to get

$$p(x_j \mid x_{j'}) \propto M_j(x_j) V_j(x_j),$$

• Computing all M_i and V_i is called the forward-backward algorithm.

Conditional Samples from Gaussian/Discrete Markov Chain

Generating exact conditional samples from Gaussian/discrete Markov chains:

- If we're only conditioning on first j states, $x_{1:j}$, just fix these values and start ancestral sampling from time (j+1).
- ② If we have the marginals $p(x_j)$, we can get the "backwards" transition probabilities using Bayes rule,

$$p(x_j \mid x_{j+1}) = \frac{p(x_{j+1} \mid x_j)p(x_j)}{p(x_{j+1})},$$

which lets us run ancestral sampling in reverse: sample x_d from $p(x_d)$, then x_{d-1} from $p(x_{d-1} \mid x_d)$, and so on.

3 If we're only conditioning on last j states $x_{d-j:d}$, run CK equations to get marginals and then start ancestral sampling "backwards" starting from (d-j-1) to sample the earlier states.

Conditional Samples from Gaussian/Discrete Markov Chain

- If we're conditioning on contiguous states in the middle, $x_{j:j'}$, run ancestral sampling forward starting from position (j'+1) and backwards starting from position (j-1).
- If you condition on non-contiguous positions j and j' with j < j', need to do (i) forward sampling starting from (j'+1), (ii) backward sampling starting from (j-1), and (iii) CK equations on the sequence (j:j') to get marginals conditioned on value of j then backwards sampling back to j starting from (j'-1).

The above are all special cases of conditioning in an undirected graphical model (UGM), followed by applying the "forward-filter backward-sampling" algorithm on each of the resulting chain-structured UGMs.