# CPSC 440/540: Advanced Machine Learning

## Markov Chains

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# Example: Vancouver Rain Data

- Consider density estimation on the "Vancouver Rain" dataset:

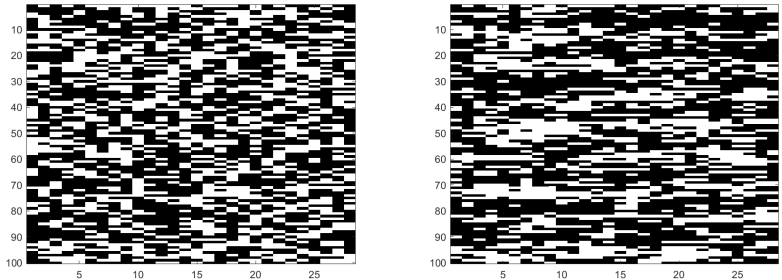
| | Day 1 | Day 2 | Day 3 | Day 4 | Day 5 | Day 6 | Day 7 | Day 8 | Day 9 | ... |
|---|---|---|---|---|---|---|---|---|---|---|
| Month 1 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 1 | 1 | |
| Month 2 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | |
| Month 3 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | |
| Month 4 | 1 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 1 | |
| Month 5 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | |
| Month 6 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 1 | 1 | |

- Variable $x_j^i = 1$ if it rained on day $j$ in month $i$.
  - Each row is a month, each column is a day of the month.
  - Data ranges from 1896-2004.

- The strongest signals in the data:
  - It tends to rain more in the winter than the summer.
  - If it rained yesterday, it's likely to rain today: $\Pr(X_j = X_{j-1}) \approx 70\%$.

# Rain Data with Product of Bernoullis

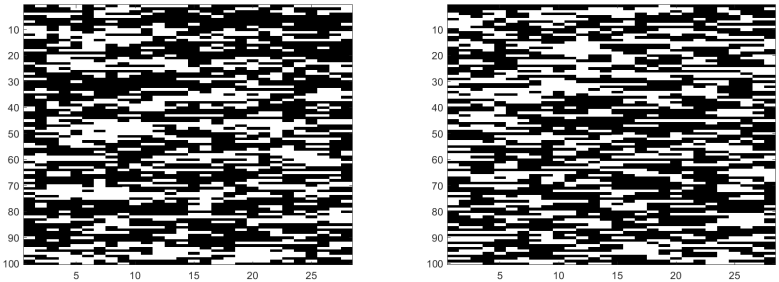
- With product of Bernoullis, we get $\Pr(X_j = \texttt{rain}) \approx 0.41$ (sadly).
  - Samples from product of Bernoullis model (left) vs. real data (right):




- Making days independent misses seasons and misses correlations.

# Markov Chains

- A better model for the between-day correlations is a Markov chain.
  - Models $\Pr(x_j \mid X_{j-1})$: probability of rain today given yesterday's value.
    - Captures dependency between adjacent days.




- It can perfectly capture the "position-independent" between-day correlation.
  - Only need a few parameters, and has a closed-form MLE.

# Markov Chain for Rain: Ingredients

- State space:
  - At time $j$, we can be in the `rain` state or the `not-rain` state.
- Initial probabilities:

| $c$ | $\Pr(X_1 = c)$ |
|---|---|
| `rain` | 0.37 |
| `not-rain` | 0.63 |

- Transition probabilities (assumed to the same for all times $j$):

| $c_{\text{old}}$ | $c_{\text{new}}$ | $\Pr(X_j = c_{\text{new}} \mid X_{j-1} = c_{\text{old}})$ |
|---|---|---|
| `rain` | `rain` | 0.65 |
| `rain` | `not-rain` | 0.35 |
| `not-rain` | `rain` | 0.25 |
| `not-rain` | `not-rain` | 0.75 |

- Because of "sum to 1" constraints, there are only 3 parameters in this model.

- We're assuming that the order of features is meaningful.
  - We're modeling dependency of each feature on the previous feature.

# Chain Rule of Probability

- By using the product rule, $p(a, b) = p(a)p(b \mid a)$, we can always decompose

$$\begin{aligned} p(x_1, x_2, \ldots, x_d) &= p(x_1)\, p(x_2, x_3, \ldots, x_d \mid x_1) \\ &= p(x_1)\, p(x_2 \mid x_1)\, p(x_3, x_4, \ldots, x_d \mid x_1, x_2) \\ &= p(x_1)\, p(x_2 \mid x_1)\, p(x_3 \mid x_2, x_1)\, p(x_4, x_5, \ldots, x_d \mid x_1, x_2, x_3), \end{aligned}$$

  and so on until we get

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

- This factorization is called the chain rule of probability.
- This turns multivariate density estimation into a sequence of univariate problems.
  - But with complicated conditioning...
  - For binary $x_j$, we'd need $2^d$ parameters for $p(x_d \mid x_1, x_2, \ldots, x_{d-1})$ alone.
  - Or we could logistic regression / neural networks / etc to estimate conditionals.

# Markov Chains

- Markov chains simplify the distribution by assuming the Markov property:

$$p(x_j \mid x_{j-1}, x_{j-2}, \ldots, x_1) = p(x_j \mid x_{j-1}),$$

  that $X_j$ is independent of the past given $X_{j-1}$.
  - "Don't care what happened 2 days ago if you know what happened yesterday".

- The probability for a sequence $x_1, x_2, \cdots, x_d$ in a Markov chain simplifies to

$$\begin{aligned} p(x_1, x_2, \ldots, x_d) &= p(x_1)\, p(x_2 \mid x_1)\, p(x_3 \mid x_2, x_1) \cdots p(x_d \mid x_{d-1}, x_{d-2}, \ldots, x_1) \\ &= p(x_1)\, p(x_2 \mid x_1)\, p(x_3 \mid x_2) \cdots p(x_d \mid x_{d-1}) \end{aligned}$$

- Another way to write this joint probability is

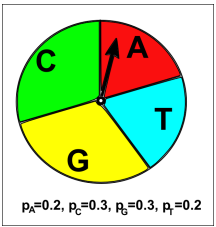
$$p(x_1, x_2, \ldots, x_d) = \underbrace{p(x_1)}_{\text{initial prob.}} \prod_{j=2}^{d} \underbrace{p(x_j \mid x_{j-1})}_{\text{transition prob.}}.$$

# Example: Modeling DNA Sequences

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

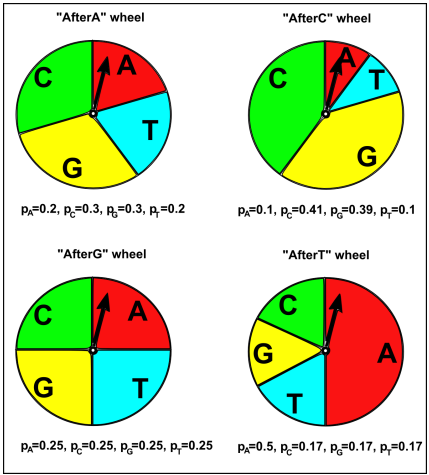
https://www.tes.com/lessons/WE5E9RncBhieAQ/dna

- Independent model for elements of sequence:



# Example: Modeling DNA Sequences

- Transition probabilities in a Markov chain model for elements of sequence:




(visualizing transition probabilities based on previous symbol):

# Markov Chains

- Markov chains are ubiquitous in sequence/time-series models:

# Homogenous Markov Chains

- For rain data it makes sense to use a homogeneous Markov chain:
  - Transition probabilities $\Pr(X_j \mid X_{j-1})$ are the same for all times $j$.

- An example of parameter tying:
  1. You have more data available to estimate each parameter.
     - Don't need to independently learn $\Pr(X_j \mid X_{j-1})$ for days 3 and 24.
  2. You can have training examples of different sizes.
     - Same model can be used for any number of days.
     - We could even treat the rain data as one long Markov chain ($n = 1$).

# Homogenous Markov Chains

- With discrete states, we could use tabular parameterization for transitions,

$$\Pr(X_j = c \mid X_{j-1} = c') = \theta_{c,c'},$$

where $\theta_{c,c'} \geq 0$ and $\sum_{c=1}^{k} \theta_{c,c'} = 1$ (and we use the same $\theta_{c,c'}$ for all $j$).

  - So we have a categorical distribution over $c$ values for each $c'$ value.

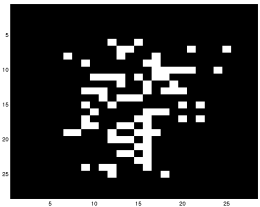
- MLE for homogeneous Markov chain with discrete $x_j$ and tabular parameters:

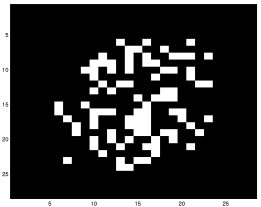
$$\theta_{c,c'} = \frac{\text{(number of transitions from } c' \text{ to } c)}{\text{(number of times we went from } c' \text{ to anything)}};$$

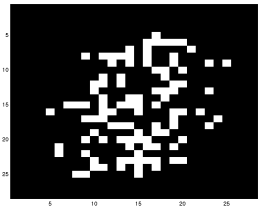
learning is just counting.

# Density Estimation for MNIST Digits

- We've previously considered density estimation for MNIST images of digits.
- We saw that product of Bernoullis does terribly



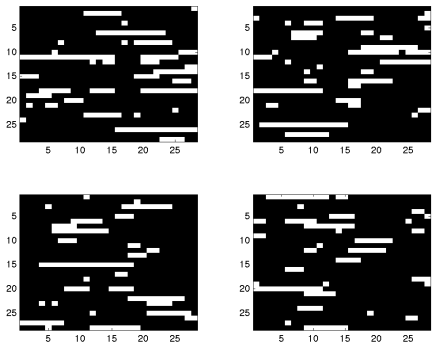




- This model misses correlation between adjacent pixels.
  - Could we capture this with a Markov chain?

# Density Estimation for MNIST Digits

- Samples from a homogeneous Markov chain (putting rows into one long vector):




- Captures correlations between adjacent pixels in the same row.
  - But misses long-range dependencies in row and dependencies between rows.
  - Also, "position independence" of homogeneity means it loses position information.

# Inhomogeneous Markov Chains

- We could allow a different $\Pr(X_j \mid X_{j-1})$ for each $j$.
  - This makes sense for digits data, but probably not for the rain data.

- For discrete $X_j$ we could use a tabular parameterization,

$$\Pr(X_j = c \mid X_{j=1} = c') = \theta^j_{c,c'}.$$

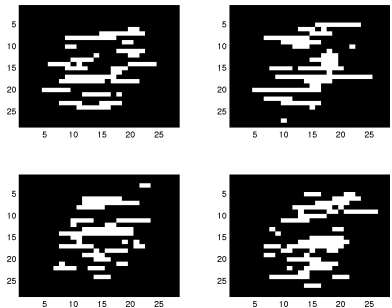
- MLE under this parameterization is given by

$$\theta^j_{c,c'} = \frac{(\text{number of transitions from } c' \text{ to } c \text{ starting at } (j-1))}{(\text{number of times we saw } c' \text{ at position } (j-1))},$$

- Inhomogeneous Markov chains include independent models as special case:
  - Use $p(x_j \mid x_{j-1}) = p(x_j)$ for all $j$; becomes a product of independent models.

# Density Estimation for MNIST Digits

- Samples from an inhomogeneous Markov chain fit to digits:




- We have correlations between adjacent pixels in rows, and position information.
  - But it isn't capturing long-range dependencies or dependency between rows.
  - Later we'll introduce graphical models to address this.

# Training Markov Chains

- Some common setups for fitting the parameters of Markov chains:
  1. We have one long sequence, and fit parameters of a homogeneous Markov chain.
     - Here, we just focus on the transition probabilities.
  2. We have many sequences of different lengths, and fit a homogeneous chain.
     - And we can use it to model sequences of any length.
  3. We have many sequences of same length, and fit an inhomgeneous Markov chain.
     - This allows "position-specific" effects.
  4. We use domain knowledge to guess the initial and transition probabilities.
     - Here we would be interested in inference in the model.

# Fun with Markov Chains

- Markov Chains "Explained Visually":
  `http://setosa.io/ev/markov-chains`
- Snakes and Ladders:
  `http://datagenetics.com/blog/november12011/index.html`
- Candyland:
  `http://www.datagenetics.com/blog/december12011/index.html`
- Yahtzee:
  `http://www.datagenetics.com/blog/january42012/`
- Chess pieces returning home and K-pop vs. ska:
  `https://www.youtube.com/watch?v=63HHmjlh794`

# Outline

# Inference in Markov Chains

- Given a Markov chain model, these are the most common inference tasks:
  1. Sampling: generate sequences that follow the probability.
  2. Marginalization: compute probability of being in state $c$ at time $j$.
  3. Stationary distribution: probability of being in state $c$ as $j$ goes to $\infty$.
     - Usually for homogeneous Markov chains.
  4. Mode decoding: compute assignment of the $x_j$ that has highest joint probability.
     - Usually for inhomogeneous Markov chains (important for supervised learning).
  5. Conditioning: do any of the above, assuming $x_j = c$ for some $j$ and $c$.
     - For example, "filling in" missing parts of a sequence.

# Ancestral Sampling

- To sample dependent random variables we can use the chain rule of probability,

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

- The chain rule suggests the following sampling strategy:
  - Sample $x_1$ from $p(x_1)$.
  - Given $x_1$, sample $x_2$ from $p(x_2 \mid x_1)$.
  - Given $x_1$ and $x_2$, sample $x_3$ from $p(x_3 \mid x_2, x_1)$.
  - ...
  - Given $x_1$ through $x_{d-1}$, sample $x_d$ from $p(x_d \mid x_{d-1}, x_{d-2}, \ldots x_1)$.

- This is called ancestral sampling.
  - It's easy if conditional probabilities are simple, since sampling in 1D is usually easy.
  - But may not be simple; binary conditional $j$ has $2^j$ values of $\{x_1, x_2, \ldots, x_j\}$.

# Ancestral Sampling Examples

- For Markov chains the chain rule simplifies to

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

- This means ancestral sampling simplifies, too:
  1. Sample $x_1$ from initial probabilities $p(x_1)$.
  2. Given $x_1$, sample $x_2$ from transition probabilities $p(x_2 \mid x_1)$.
  3. Given $x_2$, sample $x_3$ from transition probabilities $p(x_3 \mid x_2)$.
  4. ...
  5. Given $x_{d-1}$, sample $x_d$ from transition probabilities $p(x_d \mid x_{d-1})$.

# Markov Chain Toy Example: CS Grad Career

- "Computer science grad career" Markov chain:
  - Initial probabilities:

| State | Probability | Description |
|---|---|---|
| Industry | 0.60 | They work for a company or own their own company. |
| Grad School | 0.30 | They are trying to get a Masters or PhD degree. |
| Video Games | 0.10 | They mostly play video games. |

  - Transition probabilities (from row to column):

| From\to | Video Games | Industry | Grad School | Video Games (with PhD) | Industry (with PhD) | Academia | Deceased |
|---|---|---|---|---|---|---|---|
| Video Games | 0.08 | 0.90 | 0.01 | 0 | 0 | 0 | 0.01 |
| Industry | 0.03 | 0.95 | 0.01 | 0 | 0 | 0 | 0.01 |
| Grad School | 0.06 | 0.06 | 0.75 | 0.05 | 0.05 | 0.02 | 0.01 |
| Video Games (with PhD) | 0 | 0 | 0 | 0.30 | 0.60 | 0.09 | 0.01 |
| Industry (with PhD) | 0 | 0 | 0 | 0.02 | 0.95 | 0.02 | 0.01 |
| Academia | 0 | 0 | 0 | 0.01 | 0.01 | 0.97 | 0.01 |
| Deceased | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

- Here $\Pr(X_t = \text{“Grad School”} \mid X_{t-1} = \text{“Industry”}) = 0.01$.

# Example of Sampling $x_1$

- Initial probabilities are:
  - 0.1 (Video Games)
  - 0.6 (Industry)
  - 0.3 (Grad School)
  - 0 (Video Games with PhD)
  - 0 (Academia)
  - 0 (Deceased)
- So initial CDF is:
  - 0.1 (Video Games)
  - 0.7 (Industry)
  - 1 (Grad School)
  - 1 (Video Games with PhD)
  - 1 (Academia)
  - 1 (Deceased)
- To sample the initial state $x_1$:
  - First generate a number $u \sim \text{Uniform}(0, 1)$, for example $u = 0.724$.
  - Now find the first CDF value bigger than $u$, which in this case is "Grad School".

# Example of Sampling $x_2$, Given $x_1 =$ "Grad School"

- So we sampled $x_1 =$ "Grad School".
  - To sample $x_2$, we'll use the "Grad School" row in transition probabilities:

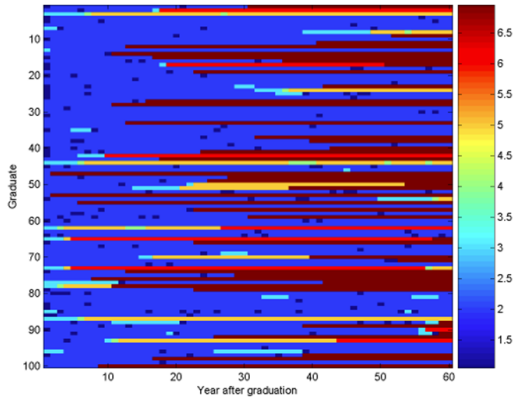
| From\to | Video Games | Industry | Grad School | Video Games (with PhD) | Industry (with PhD) | Academia | Deceased |
|---|---|---|---|---|---|---|---|
| Video Games | 0.08 | 0.90 | 0.01 | 0 | 0 | 0 | 0.01 |
| Industry | 0.03 | 0.95 | 0.01 | 0 | 0 | 0 | 0.01 |
| Grad School | 0.06 | 0.06 | 0.75 | 0.05 | 0.05 | 0.02 | 0.01 |
| Video Games (with PhD) | 0 | 0 | 0 | 0.30 | 0.60 | 0.09 | 0.01 |
| Industry (with PhD) | 0 | 0 | 0 | 0.02 | 0.95 | 0.02 | 0.01 |
| Academia | 0 | 0 | 0 | 0.01 | 0.01 | 0.97 | 0.01 |
| Deceased | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

# Example of Sampling $x_2$, Given $x_1 =$ "Grad School"

- Transition probabilities:
  - 0.06 (Video Games)
  - 0.06 (Industry)
  - 0.75 (Grad School)
  - 0.05 (Video Games with PhD)
  - 0.02 (Academia)
  - 0.01 (Deceased)
- So transition CDF is:
  - 0.06 (Video Games)
  - 0.12 (Industry)
  - 0.87 (Grad School)
  - 0.97 (Video Games with PhD)
  - 0.99 (Academia)
  - 1 (Deceased)
- To sample the second state $x_2$:
  - First generate a number $u \sim \text{Uniform}(0, 1)$, for example $u = 0.113$.
  - Now find the first CDF value bigger than $u$, which in this case is "Industry".

# Markov Chain Toy Example: CS Grad Career

- Samples from "computer science grad career" Markov chain:




- State 7 ("deceased") is called an absorbing state (no probability of leaving).
- Samples often give you an idea of what model knows (and what should be fixed).

# Ancestral Sampling with Blocks of Variables

- We sometimes factorize variables in terms of blocks of variables, as in

$$p(x_1, x_2, x_3, x_4, x_5, x_6) = p(x_1, x_2)\, p(x_3, x_4 \mid x_1, x_2)\, p(x_5, x_6 \mid x_1, x_2, x_3, x_4).$$

- With this factorization ancestral sampling takes the form
  1. Sample $x_1$ and $x_2$ from $p(x_1, x_2)$.
  2. Given $x_1$ and $x_2$, sample $x_3$ and $x_4$ from $p(x_3, x_4 \mid x_2, x_1)$.
  3. Given $x_{1:4}$, sample $x_5$ and $x_6$ from $p(x_5, x_6 \mid x_1, x_2, x_3, x_4)$.

- For example, in Gaussian discriminant analysis we write

$$p(x^i, y^i) = p(y^i)\, p(x^i \mid y^i).$$

- Sampling from Gaussian discriminant analysis:
  1. Sample $y^i$ from the categorical distribution $p(y^i)$.
  2. Sample $x^i$ from the multivariate Gaussian $p(x^i \mid y^i)$.

# Marginalization and Conditioning

- Given a density estimator, we often want to make probabilistic inferences:
  - Marginals: what is the probability that $X_j = c$?
    - What is the probability we're in industry 10 years after graduation?
  - Conditionals: what is the probability that $X_j = c$ given $X_{j'} = c'$?
    - What is the probability of industry after 10 years, if we immediately go to grad school?

- This is easy for simple independent models:
  - We directly model marginals $p(x_j)$.
  - Conditionals are marginals: $p(x_j \mid x_{j'}) = p(x_j)$.

- For Markov chains, it's more complicated.
  - $p(x_4)$ depends on the values of $x_1$, $x_2$ and $x_3$.
  - $p(x_4 \mid x_8)$ additionally depends on the values $x_5$, $x_6$, $x_7$, $x_8$.

# Monte Carlo Methods for Markov Chains

- We could use Monte Carlo approximations for inference in Markov chains:
  - Marginal $\Pr(X_j = c)$ is the number of chains that were in state $c$ at time $j$.
  - Average value at time $j$, $\mathbb{E}[X_j]$, is approximated by average of samples $x_j^i$.
  - $\Pr(5 \leq X_j \leq 10)$ is approximate by frequency of $x_j$ being between 5 and 10.
    - This makes more sense for continuous states than evaluating equalities.
  - $\Pr(x_j \leq 10, X_{j+1} \geq 10)$ is approximated by number of chains where both happen.

- Monte Carlo works for continuous states too (for inequalities and expectations).

- In typical settings Monte Carlo has slow convergence (like stochastic gradient).
  - For $\mathbb{E}[f(X)]$, the estimate $\frac{1}{n}\sum_{i=1}^{n} f(x^i)$ has variance $\mathrm{Var}(f(X))/n$.
    - If all samples look about the same ($\mathrm{Var}(f(X))$ is small), it converges quickly.
    - If samples vary a lot, it can be painfully slow.

# Exact Marginal Calculation

- For discrete-state Markov chains, we can actually compute marginals directly.
- We're given initial probabilities $\Pr(X_1 = c)$ for all $c$ as part of the definition.
- We can use transition probabilities to compute $p(x_2 = c)$ for all $c$:

$$p(x_2) = \underbrace{\sum_{x_1=1}^{k} p(x_2, x_1)}_{\text{marginalization rule}} = \sum_{x_1=1}^{k} \underbrace{p(x_2 \mid x_1)p(x_1)}_{\text{product rule}}.$$

- Same calculation gives

$$p(x_3) = \sum_{x_2=1}^{k} p(x_3, x_2) = \sum_{x_2=1}^{k} p(x_3 \mid x_2)p(x_2).$$

- So we have $p(x_3)$ in terms of $p(x_2)$, and $p(x_2)$ in terms of $p(x_1)$, which we know.

# Exact Marginal Calculation

- Recursive formula for maginals at time $j$:

$$p(x_j) = \sum_{x_{j-1}=1}^{k} p(x_j \mid x_{j-1}) p(x_{j-1}),$$

  called the Chapman-Kolmogorov (CK) equations.

- The CK equations can be implemented as matrix-vector multiplication:
  - Define $\pi^j$ as a vector containing the marginals at time $t$:

$$\pi_c^j = \Pr(X_j = c).$$

  - Define $T^j$ as a matrix cotaining the transition probabilities:

$$T_{cc'}^j = \Pr(X_j = c \mid X_{j-1} = c').$$

  - Rule is just $\pi^j = T^j \pi^{j-1}$.

# Exact Marginal Calculation

- Implementing the CK equations as a matrix multiplication:

$$T^j \pi^{j-1} = \begin{bmatrix} \Pr(X_j = 1 \mid X_{j-1} = 1) & \Pr(X_j = 1 \mid x_{j-1} = 2) & \dots & \Pr(X_j = 1 \mid x_{j-1} = k) \\ \Pr(X_j = 2 \mid X_{j-1} = 1) & \Pr(X_j = 2 \mid x_{j-1} = 2) & \dots & \Pr(X_j = 2 \mid x_{j-1} = k) \\ \Pr(X_j = k \mid X_{j-1} = 1) & \Pr(X_j = k \mid x_{j-1} = 2) & \dots & \Pr(X_j = k \mid x_{j-1} = k) \end{bmatrix} \begin{bmatrix} \Pr(X_{j-1} = 1) \\ \Pr(X_{j-1} = 2) \\ \vdots \\ \Pr(X_{j-1} = k) \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{c=1}^{k} \Pr(X_j = 1 \mid X_{j-1} = c) \Pr(X_{j-1} = c) \\ \sum_{c=1}^{k} \Pr(X_j = 2 \mid X_{j-1} = c) \Pr(X_{j-1} = c) \\ \vdots \\ \sum_{c=1}^{k} \Pr(X_j = k \mid X_{j-1} = c) \Pr(X_{j-1} = c) \end{bmatrix} = \begin{bmatrix} \Pr(X_j = 1) \\ \Pr(X_j = 2) \\ \vdots \\ \Pr(X_j = k) \end{bmatrix} = \pi^j.$$

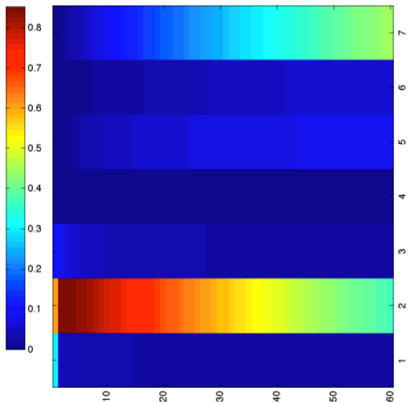
- Cost of multiplying a vector by a $k \times k$ matrix is $O(k^2)$.

- So cost to compute marginals up to time $d$ is $O(dk^2)$.
  - This is fast, considering that last step sums over all $k^d$ possible sequences.

$$p(x_d) = \sum_{x_1=1}^{k} \sum_{x_2=1}^{k} \cdots \sum_{x_{j-1}=1}^{k} \sum_{x_{j+1}=1}^{k} \cdots \sum_{x_{d-1}=1}^{k} p(x_1, x_2, \dots, x_d).$$

# Marginals in CS Grad Career

- CK equations can give all marginals $p(x_j = c)$ from CS grad Markov chain:




- Each row $j$ is a state and each column $c$ is a year.

# Continuous-State Markov Chains

bonus!

- The CK equations also apply if we have continuous states:

$$p(x_j) = \int_{x_{j-1}} p(x_j \mid x_{j-1}) p(x_{j-1}) \mathrm{d}x_{j-1},$$

  but this integral may not have a closed-form solution.

- Gaussian probabilities are an important special case:
  - If $p(x_{j-1})$ and $p(x_j \mid x_{j-1})$ are Gaussian, then $p(x_j)$ is Gaussian.
    - Marginal of product of Gaussians.
  - So we can write $p(x_j)$ in closed-form in terms of a mean and variance.
    - Also works if states are vectors, with initial/transition following multivariate Gaussian.

- If the probabilities are non-Gaussian, usually can't represent $p(x_j)$ distribution.
  - Gaussian has the special property that it is its own conjugate prior.
  - With other distributions, you're stuck using Monte Carlo or other approximations.

# Stationary Distribution

- A stationary distribution of a homogeneous Markov chain is a distribution $\pi$ with

$$\pi(c) = \sum_{c'} p(x_j = c \mid x_{j-1} = c')\pi(c') \quad \text{or equivalently} \quad \pi = T\pi.$$

- "Marginal probabilities don't change across time".
  - A stationary distribution is called an "invariant" distribution.
  - Note this does not imply it converges to a single state.

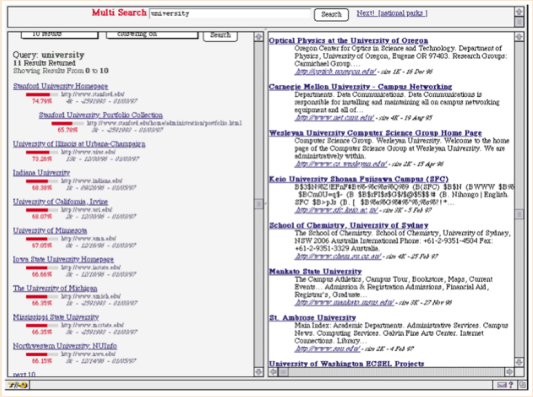
- Under certain conditions, marginals converge to a stationary distribution.
  - $p(x_j = c) \to \pi(c)$ as $j$ goes to $\infty$.
  - If we fit a Markov chain to the rain example, we have $\pi(\texttt{rain}) = 0.41$.
  - In the CS grad student example, we have $\pi(\texttt{deceased}) = 1$.

- Stationary distribution is basis for Google's PageRank algorithm.

# Application: PageRank

bonus!

- Web search before Google:



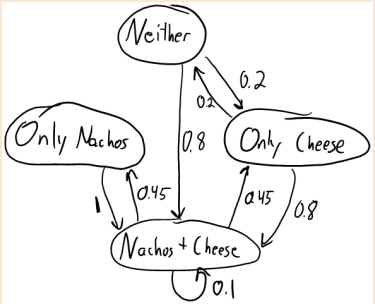

http://ilpubs.stanford.edu:8090/422/1/1999-66.pdf

- It was also easy to fool search engines by copying popular websites.

# State Transition Diagram

bonus!

- State transition diagrams are common for visualizing homogenous Markov chains:




$$T = \begin{bmatrix} 0 & 0 & 0.2 & 0.8 \\ 0 & 0 & 0 & 1 \\ 0.2 & 0 & 0 & 0.8 \\ 0 & 0.45 & 0.45 & 0.1 \end{bmatrix}$$

- Each node is a state, each edge is a non-zero transition probability.
  - For web-search, each node will be a webpage.
- Cost of CK equations is only $O(z)$ instead of $O(k^2)$ if you have only $z$ edges.

# Application: PageRank

bonus!

- Wikipedia's cartoon illustration of Google's PageRank:
  - Large face means higher rank.


https://en.wikipedia.org/wiki/PageRank

- "Important webpages are linked from other important webpages."
- "A link is more meaningful if the webpage has few links."

# Application: PageRank

bonus!

- Google's PageRank algorithm for measuring the importance of a website:
  - Stationary probability in "random surfer" Markov chain:
    - With probability $\alpha$, surfer clicks on a random link on the current webpage.
    - Otherwise, surfer goes to a completely random webpage.

- To compute the stationary distribution, they use the power method:
  - Just start with some distribution, then repeatedly apply the CK equations.
  - Iterations are faster than $O(k^2)$ due to sparsity of links.
    - Transition matrix is "sparse plus rank-1" which allows fast multiplication.
  - Can be easily parallelized.

# Application: Game of Thrones

bonus!

- PageRank can be used in other applications.
- "Who is the main character in the Game of Thrones books?"

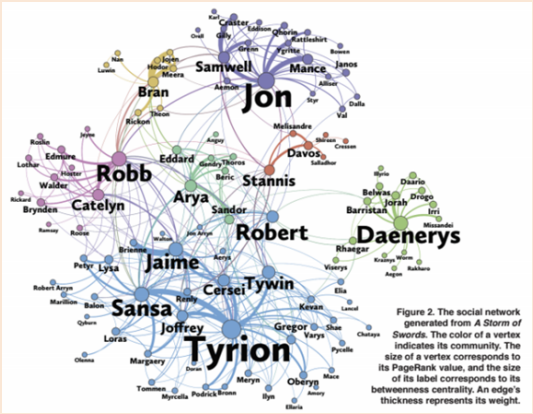



Figure 2. The social network generated from *A Storm of Swords*. The color of a vertex indicates its community. The size of a vertex corresponds to its PageRank value, and the size of its label corresponds to its betweenness centrality. An edge's thickness represents its weight.

http://qz.com/650796/mathematicians-mapped-out-every-game-of-thrones-relationship-to-find-the-main-character

# Existence/Uniqueness of Stationary Distribution

bonus!

- Does a stationary distribution $\pi$ exist and is it unique?
- Sufficient condition for existence/uniqueness: all $\Pr(x_j = c \mid x_{j'} = c') > 0$.
  - PageRank satisfies this by adding probability $(1 - \alpha)$ of jumping to a random page.
- Weaker sufficient condition for existence and uniqueness is ergodicity:
  1. "Irreducible" (doesn't get stuck in part of the graph).
  2. "Aperiodic" (probability of returning to state isn't on fixed intervals).

# Summary

- Markov chains model dependencies between adjacent features.
  - Set of possible states; initial probabilities; transition probabilities.
- Chain rule of probability.
  - Writes joint probability in terms of conditionals over "earlier" variables.
- Markov assumption.
  - Conditional independence from "past" times given previous time.
- Homogeneous Markov chains: same transition probabilities across time.
  - Allows sequences of different lengths; more data to estimate transition parameters.
- Inhomogeneous Markov chains: transition probabilities can vary.
- Ancestral sampling generates samples from multivariate distributions.
  - Use chain rule of probability, sequentially sample variables from conditionals.
- Chapman-Kolmogorov equations compute exact univariate marginals.
  - For discrete or Gaussian Markov chains.
- Stationary distribution of homogenous Markov chain.
  - Marginals as time goes to $\infty$; basis of e.g. Google's PageRank method.

- Next time: voice Photoshop.

# Label Propagation as a Markov Chain Problem

bonus!

- Semi-supervised label propagation method has a Markov chain interpretation.
  - We have $n + t$ states, one for each [un]labeled example.
- Monte Carlo approach to label propagation ("adsorption"):
  - At time $t = 0$, set the state to the node you want to label.
  - At time $t > 0$ and on a labeled node, output the label.
    - Labeled nodes are absorbing states.
  - At time $t > 0$ and on an unlabeled node $i$:
    - Move to neighbour $j$ with probability proportional $w_{ij}$ (or $\bar{w}_{ij}$).
- Final predictions are probabilities of outputting each label.
  - Nice if you only need to label one example at a time (slow if labels are rare).
  - Common hack is to limit random walk time to bound runtime.

# Outline

# Application: Voice Photoshop

bonus!

- Adobe VoCo uses decoding in a Markov chain as part of synthesizing voices:

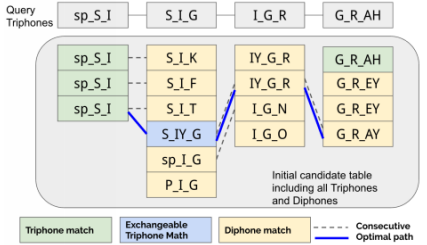



Fig. 7. Dynamic triphone preselection. For each query triphone (top) we find a candidate set of good potential matches (columns below). Good paths through this set minimize differences from the query, number and severity of breaks, and contextual mismatches between neighboring triphones.

http://gfx.cs.princeton.edu/pubs/Jin_2017_VTI/Jin2017-VoCo-paper.pdf

- https://www.youtube.com/watch?v=I3l4XLZ59iw

# Decoding: Maximizing Joint Probability

- Decoding the mode in density models: finding $x$ with highest joint probability:

$$\underset{x_1,x_2,\ldots,x_d}{\arg\max}\ p(x_1, x_2, \ldots, x_d).$$

- For CS grad student ($d = 60$) the mode is `industry` for all years.
  - The mode often doesn't look like a typical sample.
  - The mode can change if you increase $d$.

- Decoding is easy for independent models:
  - Here, $p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2)p(x_3)p(x_4)$.
  - You can optimize $p(x_1, x_2, x_3, x_4)$ by optimizing each $p(x_j)$ independently.

- Can we also maximize the marginals to decode a Markov chain?

# Example of Decoding vs. Maximizing Marginals

- Consider the "plane of doom" 2-variable Markov chain:

$$X = \begin{bmatrix} \texttt{land} & \texttt{alive} \\ \texttt{land} & \texttt{alive} \\ \texttt{crash} & \texttt{dead} \\ \texttt{explode} & \texttt{dead} \\ \texttt{crash} & \texttt{dead} \\ \texttt{land} & \texttt{alive} \\ \vdots & \vdots \end{bmatrix}.$$

- 40% of the time the plane lands and you live.
- 30% of the time the plane crashes and you die.
- 30% of the time the explodes and you die.

# Example of Decoding vs. Maximizing Marginals

- Initial probabilities are given by

$$\Pr(x_1 = \texttt{land}) = 0.4, \quad \Pr(x_1 = \texttt{crash}) = 0.3, \quad \Pr(x_1 = \texttt{explode}) = 0.3,$$

  and transition probabilites are:

$$\Pr(X_2 = \texttt{alive} \mid X_1 = \texttt{land}) = 1, \quad \Pr(X_2 = \texttt{alive} \mid X_1 = \texttt{crash}) = 0,$$
$$\Pr(X_2 = \texttt{alive} \mid X_1 = \texttt{explode}) = 0.$$

- From the CK equations, we know

$$\Pr(X_2 = \texttt{alive}) = 0.4, \quad \Pr(X_2 = \texttt{dead}) = 0.6$$

- Maximizing the marginals $p(x_j)$ independently gives (land, dead).
  - This has probability $0$, since $\Pr(\texttt{dead} \mid \texttt{land}) = 0$.

- Decoding considers the joint assignment to $x_1$ and $x_2$ maximizing probability.
  - In this case it's (land, alive), which has probability $0.4$.

# Decoding with Dynamic Programming

- Note that decoding can't be done forward in time as in CK equations.
  - Even if $\Pr(x_1 = 1) = 0.99$, the most likely sequence could have $x_1 = 2$.
  - So we need to optimize over all $k^d$ assignments to all variables.
- Fortunately, we can solve this problem using dynamic programming.
- Ingredients of dynamic programming:
  1. Optimal sub-structure.
     - We can divide the problem into sub-problems that can be solved individually.
  2. Overlapping sub-problems.
     - The same sub-problems are reused several times.

# Decoding with Dynamic Programming

- For decoding in Markov chains, we'll use the following sub-problem:
  - Compute the highest probability sequence of length $j$ ending in state $c$.
  - We'll use $M_j(c)$ as the probability of this sequence.

$$M_j(c) = \max_{x_1, x_2, \ldots, x_{j-1}} p(x_1, x_2, \ldots, x_{j-1}, c).$$

- Optimal sub-structure:
  - We can find the decoding by taking $\arg\max_{x_d} M_d(x_d)$, then backtracking.
  - Base case: $M_1(c) = \Pr(X_1 = c)$, which we're given.
  - We can compute other $M_j(s)$ recursively (derivation of this coming up),

$$M_j(s) = \max_{x_{j-1}} \underbrace{\Pr(x_j = c \mid X_{j-1} = x_{j-1})}_{\text{given}} \underbrace{M_{j-1}(x_{j-1})}_{\text{recurse}}.$$

- Overlapping sub-problems:
  - The same $k$ values of $M_{j-1}(s)$ are used to compute the $k$ values of $M_j(s)$.

# Digression: Recursive Joint Maximization

- To derive the $M_j$ formula, it will be helpful to re-write joint maximizations as

$$\max_{x_1,x_2} f(x_1,x_2) = \max_{x_1} g(x_1) \quad \text{where} \quad g(x_1) = \max_{x_2} f(x_1,x_2).$$

  - This $f_1$ "maximizes out" $x_2$, similar to marginalization rule in probability.

- Can also write this as

$$\max_{x_1,x_2} f(x_1,x_2) = \max_{x_1} \underbrace{\max_{x_2} f(x_1,x_2)}_{g(x_1)}.$$

- You can do this trick repeatedly and/or with any number of variables.

# Decoding with Dynamic Programming

- Derivation of recursive calculation for $M_j(x_j)$ for decoding Markov chains:

$$
\begin{aligned}
M_j(x_j) &= \max_{x_1,x_2,\ldots,x_{j-1}} p(x_1, x_2, \ldots, x_j) && \text{(definition of } M_j(x_j)\text{)} \\
&= \max_{x_1,x_2,\ldots x_{j-1}} p(x_j \mid x_1, x_2, \ldots x_{j-1}) p(x_1, x_2, \ldots, x_{j-1}) && \text{(product rule)} \\
&= \max_{x_1,x_2,\ldots x_{j-1}} p(x_j \mid x_{j-1}) p(x_1, x_2, \ldots, x_{j-1}) && \text{(Markov property)} \\
&= \max_{x_{j-1}} \left\{ \max_{x_1,x_2,\ldots x_{j-2}} p(x_j \mid x_{j-1}) p(x_1, x_2, x_{j-1}) \right\} && (\max_{a,b} f(a,b) = \max_a \{\max_b f(a,b)\}) \\
&= \max_{x_{j-1}} \left\{ p(x_j \mid x_{j-1}) \max_{x_1,x_2,\ldots x_{j-2}} p(x_1, x_2, x_{j-1}) \right\} && (\max_i \alpha a_i = \alpha \max_i a_i \text{ for } \alpha \geq 0) \\
&= \max_{x_{j-1}} \underbrace{p(x_j \mid x_{j-1})}_{\text{given}} \underbrace{M_{j-1}(x_{j-1})}_{\text{recurse}} && \text{(definition of } M_{j-1}(x_{j-1})\text{)}
\end{aligned}
$$

- We also store the argmax over $x_{j-1}$ for each $(j, s)$ .
  - Once we have $M_j(x_j = s)$ for all $j$ and $s$ values, backtrack using these values to solve problem.

# Example: Decoding the Plane of Doom

- We have $M_1(x_1) = p(x_1)$ so in "plane of doom" we have

$$M_1(\texttt{land}) = 0.4, \quad M_1(\texttt{crash}) = 0.3, \quad M_1(\texttt{explode}) = 0.3.$$

- We have $M_2(x_2) = \max_{x_1} p(x_2 \mid x_1) M_1(x_1)$ so we get

$$M_2(\texttt{alive}) = 0.4, \quad M_2(\texttt{dead}) = 0.3.$$

- $M_2(2) \neq p(x_2 = 2)$ because we needed to choose either `crash` or `explode`.
  - And notice that $\sum_{c=1}^{k} M_2(x_j = c) \neq 1$ (this is not a distribution over $x_2$).

- We maximize $M_2(x_2)$ to find that the optimal decoding ends with `alive`.
  - We now need to backtrack to find the state that led to `alive`, giving `land`.

# Viterbi Decoding

- The Viterbi decoding dynamic programming algorithm:
  1. Set $M_1(x_1) = p(x_1)$ for all $x_1$.
  2. Compute $M_2(x_2)$ for all $x_2$, store argmax of $x_1$ leading to each $x_2$.
  3. Compute $M_3(x_3)$ for all $x_3$, store argmax of $x_2$ leading to each $x_3$.
  4. ...
  5. Maximize $M_d(x_d)$ to find value of $x_d$ in a decoding.
  6. Bactrack to find the value of $x_{d-1}$ that led to this $x_d$.
  7. Backtrack to find the value of $x_{d-2}$ that led to this $x_{d-1}$.
  8. ...
  9. Backtrack to find the value of $x_1$ that led to this $x_2$.

- For a fixed $j$, computing all $M_j(x_j)$ given all $M_{j-1}(x_{j-1})$ costs $O(k^2)$.
  - Total cost is only $O(dk^2)$ to search over all $k^d$ paths.
  - Has numerous applications, like decoding digital TV.

# Viterbi Decoding

- What Viterbi decoding data structures might look like ($d = 4, k = 3$):

$$M = \begin{bmatrix} 0.25 & 0.25 & 0.50 \\ 0.35 & 0.15 & 0.05 \\ 0.10 & 0.05 & 0.05 \\ 0.02 & 0.03 & 0.05 \end{bmatrix}, \quad B = \begin{bmatrix} \emptyset & \emptyset & \emptyset \\ 1 & 1 & 3 \\ 2 & 1 & 1 \\ 2 & 2 & 1 \end{bmatrix}.$$

- The $d \times k$ matrix $M$ stores the values $M_j(s)$, while $B$ stores the argmax values.

- From the last row of $M$ and the backtracking matrix $B$, the decoding is $x_1 = 1, x_2 = 2, x_3 = 1, x_4 = 3$.

# Conditional Probabilities in Markov Chains: Easy Case

- How do we compute conditionals like $\Pr(x_j = c \mid x_{j'} = c')$ in Markov chains?

- Consider conditioning on an earlier time, like computing $p(x_{10} \mid x_3)$:
  - We are given the value of $x_3$.
  - We obtain $p(x_4 \mid x_3)$ by looking it up among transition probabilities.
  - We can compute $p(x_5 \mid x_3)$ by adding conditioning to the CK equations,

$$
\begin{aligned}
p(x_5 \mid x_3) &= \sum_{x_4} p(x_5, x_4 \mid x_3) && \text{(marg rule)} \\
&= \sum_{x_4} p(x_5 \mid x_4, x_3) p(x_4 \mid x_3) && \text{(product rule)} \\
&= \sum_{x_4} \underbrace{p(x_5 \mid x_4)}_{\text{given}} \underbrace{p(x_4 \mid x_3)}_{\text{recurse}} && \text{(Markov property).}
\end{aligned}
$$

  - Repeat this to find $p(x_6 \mid x_3)$, then $p(x_7 \mid x_3)$, up to $p(x_{10} \mid x_3)$.

# Conditional Probabilities in Markov Chains with "Forward" Messages

- How do we condition on a future time, like computing $p(x_3 \mid x_6)$?
  - Need to sum over "past" values $x_1$ and $x_2$, and "future" values $x_4$ and $x_5$.

$$
\begin{aligned}
p(x_3 \mid x_6) \propto p(x_3, x_6) &= \sum_{x_5}\sum_{x_4}\sum_{x_2}\sum_{x_1} p(x_1, x_2, x_3, x_4, x_5, x_6) \quad \text{(cond. prob. and marg. rule)} \\
&= \sum_{x_5}\sum_{x_4}\sum_{x_2}\sum_{x_1} p(x_6 \mid x_5)p(x_5 \mid x_4)p(x_4 \mid x_3)p(x_3 \mid x_2)p(x_2 \mid x_1)p(x_1) \\
&= \sum_{x_5} p(x_6 \mid x_5) \sum_{x_4} p(x_5 \mid x_4)p(x_4 \mid x_3) \sum_{x_2} p(x_3 \mid x_2) \sum_{x_1} p(x_2 \mid x_1)p(x_1) \\
&= \sum_{x_5} p(x_6 \mid x_5) \sum_{x_4} p(x_5 \mid x_4)p(x_4 \mid x_3) \sum_{x_2} p(x_3 \mid x_2)M_2(x_2) \\
&= \sum_{x_5} p(x_6 \mid x_5) \sum_{x_4} p(x_5 \mid x_4)p(x_4 \mid x_3)M_3(x_3) \\
&= \sum_{x_5} p(x_6 \mid x_5)M_5(x_5) \\
&= M_6(x_6) \quad \text{(the values } M_j \text{ are called "forward messages")}
\end{aligned}
$$

- $M_j(x_j)$ summarizes "everything you need to know up to time $j$ for this $x_j$ value".
  - Different $x_3$ will give different $M_6$ values; normalize these to get final result.

# Conditional Probabilities in Markov Chains with "Backward" Messages

- We could exchange order of sums to do computation "backwards" in time:

$$
\begin{aligned}
p(x_3 \mid x_6) &= \sum_{x_1}\sum_{x_2}\sum_{x_4}\sum_{x_5} p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2)p(x_4 \mid x_3)p(x_5 \mid x_4)p(x_6 \mid x_5) \\
&= \sum_{x_1} p(x_1) \sum_{x_2} p(x_2 \mid x_1)p(x_3 \mid x_2) \sum_{x_4} p(x_4 \mid x_3) \sum_{x_5} p(x_5 \mid x_4)p(x_6 \mid x_5) \\
&= \sum_{x_1} p(x_1) \sum_{x_2} p(x_2 \mid x_1)p(x_3 \mid x_2) \sum_{x_4} p(x_4 \mid x_3)V_4(x_4) \\
&= \sum_{x_1} p(x_1) \sum_{x_2} p(x_2 \mid x_1)p(x_3 \mid x_2)V_3(x_3) \\
&= \sum_{x_1} p(x_1)V_1(x_1) \quad \text{(the values } V_j \text{ are called "backward messages")}
\end{aligned}
$$

- The $V_j$ summarize "everything you need to know after time $j$ for this $x_j$ value".
  - Sometimes called "cost to go" function, as in "what is the cost for going to $x_j$."
  - Sometimes called a value function, as in "what is the future value of being in $x_j$."

# Motivation for Forward-Backward Algorithm

- Why do care about being able to solve this "forward" or "backward" in time?
  - Cost is $O(dk^2)$ in both directions to compute conditionals in Markov chains.
- Consider computing $p(x_1 \mid A)$, $p(x_2 \mid A)$,..., $p(x_d \mid A)$ for some event $A$.
  - Need all these conditionals to add features, compute conditionals with neural networks, or partial observations (as in hidden Markov models, HMMs).
- We could solve this in $O(dk^2)$ for each time, giving a total cost of $O(d^2k^2)$.
  - Using forward messages $M_j(x_j)$ at each time, or backwards messages $V_j(x_j)$.
- Alternately, the forward-backward algorithm computes all conditionals in $O(dk^2)$.
  - By doing one "forward" pass and one "backward" pass with appropriate messages.

# Potential Function Representation of Markov Chains

- Forward-backward algorithm considers probabilities written in the form

$$p(x_1, x_2, \ldots, x_d) = \frac{1}{Z}\left(\prod_{j=1}^{d} \phi_j(x_j)\right)\left(\prod_{j=2}^{d} \psi_j(x_j, x_{j-1})\right).$$

- The $\phi_j$ and $\psi_j$ functions are called potential functions.
  - They can map from a state ($\phi$) or two states ($\psi$) to a non-negative number.
  - Normalizing constant $Z$ ensures we sum/integrate to 1 (over all $x_1$, $x_2$,...,$x_d$).

- We can write Markov chains in this form by using (in this case $Z = 1$):
  - $\phi_1(x_1) = p(x_1)$ and $\phi_j(x_j) = 1$ when $j \neq 1$.
  - $\psi_j(x_{j-1}, x_j) = p(x_j \mid x_{j-1})$.

- Why do we need the $\phi_j$ functions?
  - To condition on $x_j = c$, set $\phi_j(c) = 1$ and $\phi_j(c') = 0$ for $c' \neq c$.
  - For "hidden Markov models" (HMMs), the $\phi_j$ will be the "emission probabilities".
  - For neural networks, $\phi_j$ will be $\exp$(neural network output) (generalizes softmax).

# Forward-Backward Algorithm

- Forward pass in forward-backward algorithm (generalizes CK equations):
  - Set each $M_1(x_1) = \phi_1(x_1)$.
  - For $j = 2$ to $j = d$, set each $M_j(x_j) = \sum_{x_{j-1}} \phi_j(x_j)\psi_j(x_j, x_{j-1})M_{j-1}(x_{j-1})$.
    - "Multiply by new terms at time $j$, summing up over $x_{j-1}$ values."

- Backward pass in forward-backward algorithm:
  - Set each $V_d(x_d) = \phi_d(x_d)$.
  - For $(d-1)$ to $j = 1$, set each $V_j(x_j) = \sum_{x_{j+1}} \phi_j(x_j)\psi_{j+1}(x_{j+1}, x_j)V_{j+1}(x_{j+1})$.

- We then have that $p(x_j) \propto \frac{M_j(x_j)V_j(x_j)}{\phi_j(x_j)}$.
  - Not obvious; see bonus for how it gives conditional in Markov chain.
  - We divide by $\phi_j(x_j)$ since it is included in both the forward and backward messages.
    - You can alternately shift $\phi_j$ to earlier/later message to remove division.
- We can also get the normalizing constant as $Z = \sum_{c=1}^{k} M_d(c)$.

# Forward-Backward for Decoding and Sampling

bonus!

- Viterbi decoding can be generalized to use potentials $\phi$ and $\psi$:
  - Compute forward messages, but with summation replaced by maximization:

$$M_j(x_j) \propto \max_{x_{j-1}} \phi_j(x_j)\psi_j(x_j, x_{j-1})M_{j-1}(x_{j-1}).$$

  - Find the largest value of $M_d(x_d)$, then backtrack to find decoding.

- Forward-filter backward-sample is a potentials ($\phi$ and $\psi$) variant for sampling.
  - Forward pass is the same.
  - Backward pass generates samples (ancestral sampling backwards in time):
    - Sample $x_d$ from $M_d(x_d) = p(x_d)$.
    - Sample $x_{d-1}$ using $M_{d-1}(x_{d-1})$ and sampled $x_d$.
    - Sample $x_{d-2}$ using $M_{d-2}(x_{d-2})$ and sampled $x_{d-1}$.
    - (continue until you have sampled $x_1$)