CPSC 540: Machine Learning

Message Passing

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Last Time: Monte Carlo Methods

- If we want to approximate expectations of random functions,

$$\underbrace{\mathbb{E}[g(x)] = \sum_{x \in \mathcal{X}} g(x)p(x)}_{\text{discrete } x} \quad \text{or} \quad \underbrace{\mathbb{E}[g(x)] = \int_{x \in \mathcal{X}} g(x)p(x)dx,}_{\text{continuous } x}$$

  the Monte Carlo estimate is

$$\mathbb{E}[g(x)] \approx \frac{1}{n}\sum_{i=1}^{n} g(x^i),$$

  where the x^i are independent samples from $p(x)$.

- We can use this to approximate marginals,

$$p(x_j = c) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{I}[x_j^i = c].$$

Exact Marginal Calculation

- In typical settings Monte Carlo has sublinear converngece like stochastic gradient.
  - Speed affected is measured by variance of samples.
    - If all samples look the same, it converges quickly.
    - If samples look very different, it can be painfully slow.

- We can sometimes avoid Monte Carlo and compute univariate marginals exactly:
  - Markov chains with discrete or Gaussian probabilities.

- In the discrete case, we're giving $p(x_1)$ and we can compute $p(x_2)$ using:

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

- We can repeat this calculation to obtain $p(x_3)$ and other subsequent marginals.

Exact Marginal Calculation

- Recursive marginal formula is called the Chapman-Kolmogorov (CK) equations:

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

- CK equations for one x_j costs $O(k)$.
- To compute $p(x_j)$ for all k states costs $O(k^2)$.
  - Can be written as matrix-vector product with $k \times k$ transition probabilities matrix.

- With CK equations, computing all marginals costs $O(dk^2)$.

Continuous-State Markov Chains

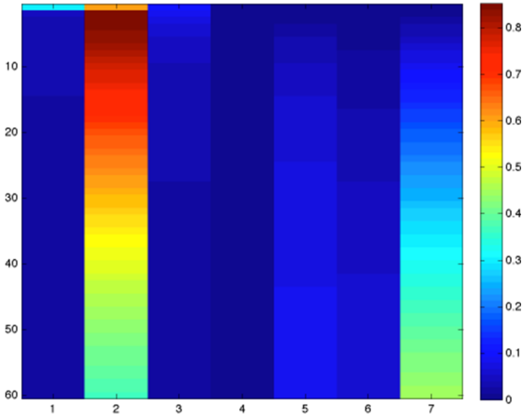
- The CK equations also apply if we have continuous states:

$$p(x_j) = \int_{x_{j-1}} p(x_j \mid x_{j-1})p(x_{j-1}).$$

- 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.
  - So we can write $p(x_j)$ in closed-form in terms of mean and variance.
- If the probabilities are non-Gaussian, usually can't represent $p(x_j)$ distribution.
  - You are stuck using Monte Carlo or other approximations.

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 year and each column c is a state.

Stationary Distribution

- A stationary distribution of a homogeneous Markov chain is a vector π satisfying

$$\pi(c) = \sum_{c'} p(x_j = c \mid x_{j-1} = c')\pi(c').$$

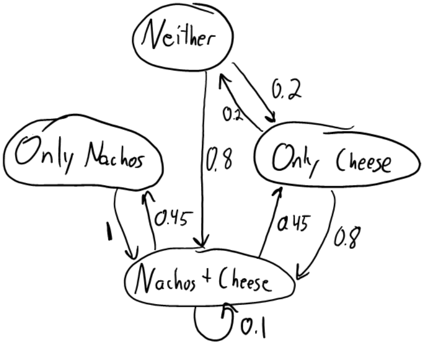
- "The probabilities don't change across time" (also called "invariant" distribution).

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

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

State Transition Diagram

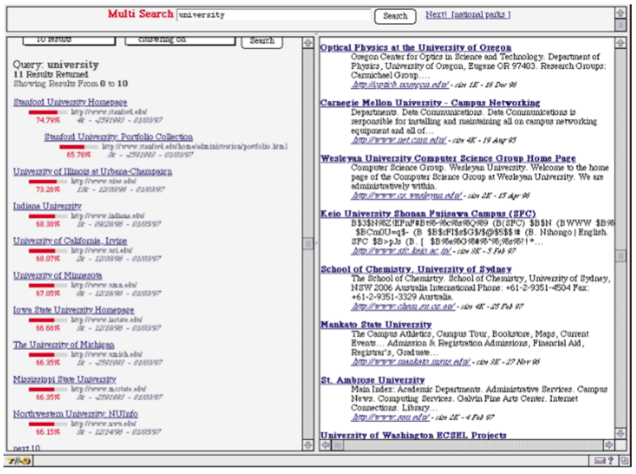
- State transition diagrams are common for visualizing homogenous Markov chains:



- Each node is a state, each edge is a non-zero transition probability.
- Cost of CK equations is only $O(z)$ if you have only z edges.

Application: PageRank

- Web search before Google:



Query: **university**
11 Results Returned
Showing Results From **0** to **10**

Stanford University Homepage
http://www.stanford.edu/
74.79%

Stanford University: Portfolio Collection
http://www.stanford.edu/home/administration/portfolio.html
65.78%

University of Illinois at Urbana-Champaign
http://www.uiuc.edu/
73.26%

Indiana University
http://www.indiana.edu/
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67.05%

Iowa State University Homepage
http://www.iastate.edu/
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next 10

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Oregon Center for Optics in Science and Technology. Department of Physics, University of Oregon, Eugene OR 97403. Research Groups: Carmichael Group....
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Departments. Data Communications. Data Communications is responsible for installing and maintaining all on campus networking equipment and all of...
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University of Washington ECSEL Projects

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

Application: PageRank

- 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".
- "Link is more meaningful if a webpage has few links".

Application: PageRank

- Google's PageRank algorithm for measuring the importance of a website:
    - Stationary probability in "random surfer" Markov chain:
        - With probability α, 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:
    - Repeatedly apply the CK equations.
    - Iterations are faster than $O(k^2)$ due to sparsity of links.
    - Can be easily parallelized.
    - Achieves a linear convergence rate.

- More recent works have shown coordinate optimization can be faster.

Application: Game of Thrones

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

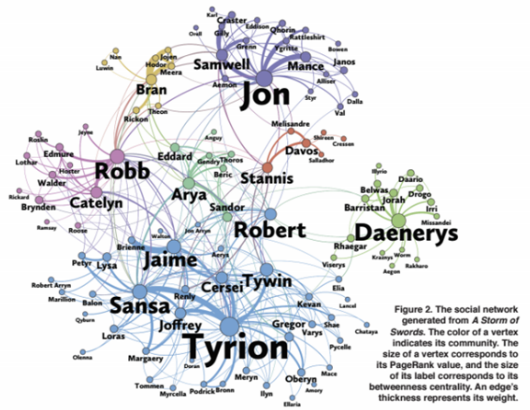

Figure 2. The social network generated from *A Storm of Swords*. The color of a vertex indicates its community. The size of a vertex corresponds to its PageRank value, and the size of its label corresponds to its betweenness centrality. An edge's thickness represents its weight.

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

Existence/Uniqueness of Stationary Distribution

- Does a stationary distribution π exist and is it unique?
- A sufficient condition for existence/uniqueness is that all $p(x_j = c \mid x_{j'} = c') > 0$.
    - PageRank adds probability α of jumping to a random page.
- Weaker sufficient conditions for existene and uniqueness ("ergodic"):
    1. "Irreducible" (doesn't get stuck in part of the graph).
    2. "Aperiodic" (probability of returning to state isn't on fixed intervals).

Outline

Decoding: Maximizing Joint Probability

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

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

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

- Decoding is easy for independent models:
  - We can just optimize each x_j independently.
  - For example, with four variables we have

$$\max_{x_1,x_2,x_3,x_4}\{p(x_1)p(x_2)p(x_3)p(x_4)\} = \left(\max_{x_1} p(x_1)\right)\left(\max_{x_2} p(x_2)\right)\left(\max_{x_3} p(x_3)\right)\left(\max_{x_4} p(x_4)\right).$$

- 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:

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

- Initial probabilities are given by

$$p(x_1 = \text{“land”}) = 0.4, \quad p(x_1 = \text{“crash”}) = 0.3, \quad p(x_1 = \text{“explode”}) = 0.3,$$

and x_2 is "alive" iff x_1 is "land".

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  and x_2 is “alive” iff x_1 is “land”.

- If we apply the CK equations we get

$$p(x_2 = \text{‘’alive”}) = 0.4, \quad p(x_2 = \text{“dead”}) = 0.6,$$

  so maximizing the marginals $p(x_j)$ independently gives (“land”, “dead”).
    - This actually has probability 0.

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

Distributing Max across Product

- Note that decoding can't be done forward in time as in CK equations.
  - We need to optimize over all k^d assignments to all variables.
  - Even if $p(x_1 = 1) = 0.99$, the most likely sequence could have $x_1 = 2$.

- Fortunately, the Markov property makes the max simplify:

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

where we're using that $\max_i \alpha a_i = \alpha \max_i a_i$ for non-negative α.

Decoding with Memoization

- The Markov property writes decoding as a sequence of max problems:

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

but note that we can't just "solve" $\max_{x_1}$ once because it's a function of x_2.

  - Instead, we'll memoize solution $M_2(x_2) = \max_{x_1} p(x_2 \mid x_1)p(x_1)$ for all x_2,

$$\max_{x_1,x_2,x_3,x_4} p(x_1,x_2,x_3,x_4) = \max_{x_4}\max_{x_3} p(x_4 \mid x_3)\max_{x_2} p(x_3 \mid x_2)M_2(x_2).$$

- Now we memoize solution $M_3(x_3) = \max_{x_2} p(x_3 \mid x_2)M_2(x_2)$ for all x_3,

$$\max_{x_1,x_2,x_3,x_4} p(x_1,x_2,x_3,x_4) = \max_{x_4}\max_{x_3} p(x_4 \mid x_3)M_3(x_3).$$

- And defining $M_4(x_4) = \max_{x_3} p(x_4 \mid x_3)M_2(x_3)$ the maximum value is given by

$$\max_{x_1,x_2,x_3,x_4} p(x_1,x_2,x_3,x_4) = \max_{x_4} M_4(x_4).$$

Example: Decoding the Plane of Doom

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

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

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

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

- $M_2(2) \neq p(x_2 = 2)$ because we needed to choose either "crash" or "explode".
- We maximize $M_2(x_2)$ to find that optimal decoding ednds with "alive".
  - We now need to backtrack to find the state that lead to "alive", giving "land".

Viterbi Decoding

- What is $M_j(x_j)$ in words?
    - "Probability of most likely length-j sequence ending in x_j (ignoring future)".

- The Viterbi decoding algorithm (special case of dynamic programming):
    1. Set $M_1(x_1) = p(x_1)$ for all x_1.
    2. Compute $M_2(x_2)$ for all x_2, store value of x_1 leading to the best value of each x_2.
    3. Compute $M_3(x_3)$ for all x_3, store value of x_2 leading to the best value of 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 lead to this x_d.
    7. Backtrack to find the value of x_{d-2} that lead to this x_{d-1}.
    8. ...

- 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.

Application: Voice Photoshop

- Application: Adobe VoCo uses Viterbi as part of synthesizing voices:

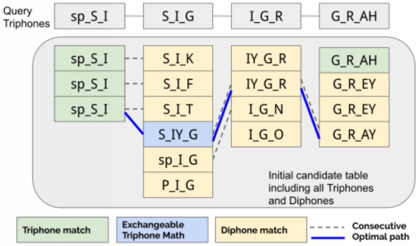

Fig. 7. Dynamic triphone preselection. For each query triphone (top) we find a candidate set of good potential matches (columns below). Good paths through this set minimize differences from the query, number and severity of breaks, and contextual mismatches between neighboring triphones.

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

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

Summary

- Chapman-Kolmogorov equations compute exact univariate marginals.
    - For discrete or Gaussian Markov chains.
- Stationary distribution of homogenous Markov chain.
    - Marginals as time goes to ∞.
    - Basis of Google's PageRank method.
- Decoding is task of finding most probable x.
- Viterbi decoding allow efficient decoding with Markov chains.
- Next time: weakening the Markov assumption.