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,

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

Exact Marginal Calculation

- In typical settings Monte Carlo has slow convergence like stochastic gradient.
  - $O(1/t)$ convergence rate where constant is variance of samples.
    - If all samples look the same, it converges quickly.
    - If samples look very different, it can be painfully slow.

- For discrete-state Markov chains, we can actually compute marginals directly:
  - We're given initial probabilities $p(x_1 = s)$ for all s as part of the definition.
  - We can use transition probabilities to compute $p(x_2 = s)$ for all s:

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

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

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 π^j as a vector containing the marginals at time t:

$$\pi_c^j = p(x_j = c).$$

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

$$T_{cc'}^j = p(x_j = c \mid x_{j-1} = c').$$

Exact Marginal Calculation

- Implementing the CK equations as a matrix multiplications:

$$T^j \pi^{j-1} = \begin{bmatrix} p(x_j = 1 | x_{j-1} = 1) & p(x_j = 1 | x_{j-1} = 2) & \dots & p(x_j = 1 | x_{j-1} = k) \\ p(x_j = 2 | x_{j-1} = 1) & p(x_j = 2 | x_{j-1} = 2) & \dots & p(x_j = 2 | x_{j-1} = k) \\ p(x_j = k | x_{j-1} = 1) & p(x_j = k | x_{j-1} = 2) & \dots & p(x_j = k | x_{j-1} = k) \end{bmatrix} \begin{bmatrix} p(x_{j-1} = 1) \\ p(x_{j-1} = 2) \\ \vdots \\ p(x_{j-1} = k) \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{c=1}^k p(x_j = 1 \mid x_{j-1} = c) p(x_{j-1} = c) \\ \sum_{c=1}^k p(x_j = 2 \mid x_{j-1} = c) p(x_{j-1} = c) \\ \vdots \\ \sum_{c=1}^k p(x_j = k \mid x_{j-1} = c) p(x_{j-1} = c) \end{bmatrix} = \begin{bmatrix} p(x_j = 1) \\ p(x_j = 2) \\ \vdots \\ p(x_j = k) \end{bmatrix} = \pi^j.$$

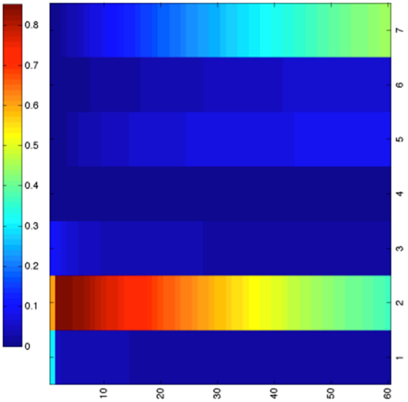
- Cost of multiplying a vector by a $k \times k$ matrix is $O(k^2)$.

- 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 paths.

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

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

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

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

  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.
    - Joint distribution is a product of Gaussians.
  - 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.

Stationary Distribution

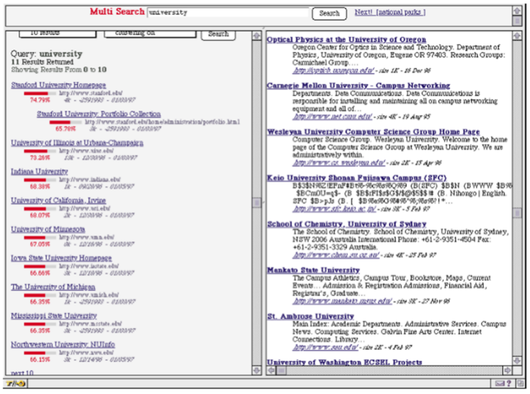
- A stationary distribution of a homogeneous Markov chain is a vector π satisfying

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

- "Probabilities don't change across time" (also called "invariant" distribution).
  - Here are talking about the "marginal" probabilities $p(x_j)$, not the "transition" probabilities $p(x_j \mid x_{j-1})$.
- 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.

Application: PageRank

- Web search before Google:

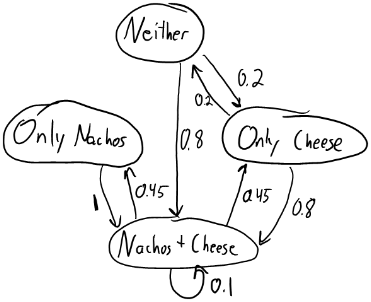


http://ilpubs.stanford.edu:8090/422/1/1999-66.pdf

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

State Transition Diagram

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



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

- 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 $O(z)$ if you have only z edges.

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.
    - Transition matrix is "sparse plus rank-1" which allows fast multiplication.
  - Can be easily parallelized.

Application: Game of Thrones

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

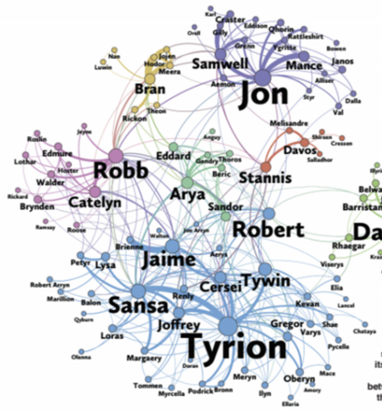


Figure 2. The social network generated from *A Storm of Swords*. The color of a vertex indicates its community. The size of a vertex corresponds to its PageRank value, and the size of its label corresponds to its betweenness centrality. An edge's thickness represents its weight.

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 satisfies this by adding probability α of jumping to a random page.
- Weaker sufficient conditions for existence 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:

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

- 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:
    - 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:

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

- 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

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

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

- 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.

Digression: Recursive Joint Maximization

- To decode Markov chains, it will be helpful to re-write joint maximizations as

$$\max_{x_1,x_2} f(x_1,x_2) = \max_{x_1} f_1(x_1),$$

  where $f_1(x_1) = \max_{x_2} f(x_1,x_2)$ (this f_1 "maximizes out" over x_2).
  - This is similar to the marginalization rule in probability.

- Plugging in the definition of $f_1(x_1)$ we obtain:

$$\max_{x_1,x_2} f(x_1,x_2) = \max_{x_1} \underbrace{\max_{x_2} f(x_1,x_2)}_{f_1(x_1)}.$$

Decoding with Dynamic Programming

- Note that decoding can't be done forward in time as in CK equations.
  - Even if $p(x_1 = 1) = 0.99$, 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.

- Key quantity is solving the sub-problem $M_j(x_j)$.
  - Find the "highest probability sequence of length j ending in x_j",

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

  - Base case: $M_1(x_1) = p(x_1)$ (which is given by the initial probability).
  - We can compute other $M_j(x_j)$ recursively (next slide).

Decoding with Dynamic Programming

- Recursive calculation of "highest probability sequence of length j ending in x_j":

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

- Once we have computed $M_j(x_j = c)$ for all j and c values, we can backtrack to solve the problem (later).

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".
  - 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 lead to "alive", giving "land".

Viterbi Decoding

- 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. ...
  9. Backtrack to find the value of x_1 that lead to this x_2.

- 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.

Application: Voice Photoshop

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

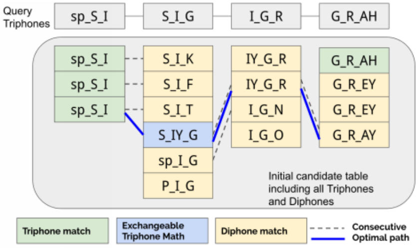


Fig. 7. Dynamic triphone preselection. For each query triphone (top) we find a candidate set of good potential matches (columns below). Good paths through this set minimize differences from the query, number and severity of breaks, and contextual mismatches between neighboring triphones.

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: measuring defence in the NBA.

Label Propagation as a Markov Chain Problem

- Basic 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.