COMPSCI 614: Randomized Algorithms with Applications to Data Science

Prof. Cameron Musco

University of Massachusetts Amherst. Spring 2024.

Lecture 22

Logistics

- Optional Problem Set 5 due 5/13 at 11:59pm.
- Final exam will be Tuesday 5/14, 10:30-12:30pm in the classroom. Study materials to be posted soon.
- Final project due the last day of finals: Friday 5/17.

Summary

Last Time:

- Finish up coupling. Example applications to shuffling, random walks on hypercubes, and exponential convergence of TV distance. $\tau(\varepsilon) \lesssim \tau(c) \cdot \log(1/\varepsilon)$ $\quad c < 1/2$
- Markov Chain Monte Carlo – example of sampling random independent sets.
- Start on Metropolis Hastings algorithms and application to sampling from the hardcore model.

Summary

Last Time:

- Finish up coupling. Example applications to shuffling, random walks on hypercubes, and exponential convergence of TV distance.
- Markov Chain Monte Carlo – example of sampling random independent sets.
- Start on Metropolis Hastings algorithms and application to sampling from the hardcore model.

Today:

- Finish the Metropolis Hastings algorithm.
- Sampling to counting reduction for independent sets.

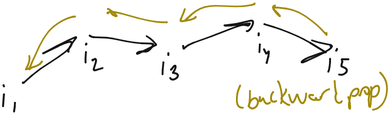
Mixing Time and Eigenvalues

A Markov chain is reversible if $\pi(i)P_{ij} = \pi(j)P_{ji}$ for all i, j. I.e., if the probability of transitioning from state i to state j is equal to the probability of transitioning from state j to state i in the steady state distribution. 'Detailed balance' condition.

- symmetric chain $P_{ij} = P_{ji} \Rightarrow \pi(i) = \pi(j)$ reversible trivially
- random walk on undirected graph.

$\pi(i)\cdot P_{ij} = \frac{d_i}{2|E|}\cdot\frac{1}{d_i} = \frac{1}{2|E|}$ $\quad \pi(j)P_{ji} = \frac{d_j}{2|E|}\cdot\frac{1}{d_j} = \frac{1}{2E}$

$=$



$\pi(1)\cdot P_{12}\cdot P_{23}\cdots P_{45}$ (forward probability)

$\pi(1)\cdot\frac{\pi(2)}{\pi(1)}\cdot P_{21}\cdot\frac{\pi(3)}{\pi(2)}\cdot P_{32}\cdots\frac{\pi(5)}{\pi(4)}\cdot P_{54}$

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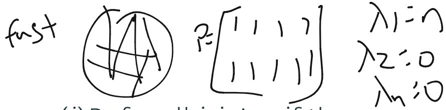
- If the chain is irreducible and reversible, P has all real eigenvalues, $1 = \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \geq -1$

$$\pi P = \pi$$

Mixing Time and Eigenvalues



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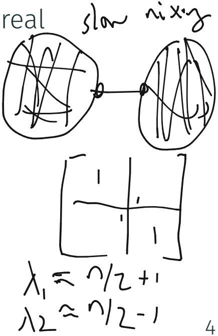
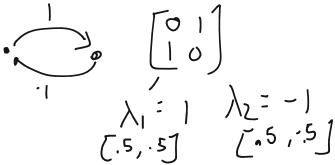
- If the chain is irreducible and reversible, P has all real eigenvalues, $1 = \lambda_1 > \lambda_2 \ldots > \lambda_n$.
- The eigenvalue gap is $\gamma = \lambda_1 - \max\{|\lambda_2|, |\lambda_n|\}$.
- The mixing time is equal to $\tau(\epsilon) = \tilde{O}(\frac{1}{\gamma})$.

$\leq O\left(\frac{\log(1/\epsilon)}{\gamma}\right)$





Mixing Time and Eigenvalues

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$$\frac{\pi(i)^{1/2} P_{ij}}{\pi(j)^{1/2}} = \frac{\pi(j)^{1/2} P_{ji}}{\pi(i)^{1/2}}$$

Proof:

$D^{1/2} P D^{-1/2}$

- Let $D = diag(\pi)$. Then $D^{1/2}PD^{-1/2}$ is symmetric (and thus has real eigenvalues)

M

$$m_{ij} = D_{ii}^{1/2} \cdot P_{ij} \cdot D_{jj}^{-1/2} = \frac{\pi(i)^{1/2}}{\pi(j)^{1/2}} \cdot P_{ij} \qquad m_{ji} = \frac{\pi(j)^{1/2}}{\pi(i)^{1/2}} P_{ji}$$

detailed balance

Mixing Time and Eigenvalues

Claim: If a Markov chain is reversible (i.e., $\pi(i)P_{ij} = \pi(j)P_{ji}$ for all i, j), then P has all real eigenvalues.

Proof:

- Let $D = diag(\pi)$. Then $D^{-1/2}PD^{1/2}$ is symmetric (and thus has real eigenvalues)
- The above is a similarity transform. The eigenvalues of P are identical to the eigenvalues of $D^{-1/2}PD^{1/2}$ and are thus real.

$A^T A = A^2$

$v^T A^T A v$ $\|Av\|_2^2$ which is nonnegative

$v^T A^2 v = v^T \lambda^2 v = \lambda^2 \|v\|_2^2$ λ^2 is nonnegative real.

how to prove symmetric matrix has real eigs?

MCMC Methods Continued

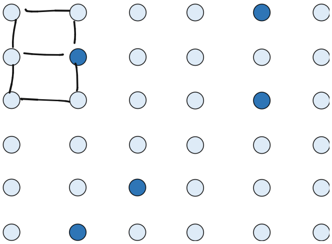
Achieving a Non-Uniform Stationary Distribution

Suppose we want to sample an independent set X from our graph with probability:

$$\pi(X) = \frac{\lambda^{|X|}}{\sum_{Y \text{ independent}} \lambda^{|Y|}},$$

for some 'fugacity' parameter $\lambda > 0$.

Known as the 'hard-core model' in statistical physics.



Metropolis-Hastings Algorithm

A very generic way of designing a Markov chain over state space $[m]$ with stationary distribution $\pi \in [0,1]^m$.

- Assume the ability to efficiently compute a density $p(X) \propto \pi(X)$.
- Assume access to some symmetric transition function with transition probability matrix $Q \in [0,1]^{m \times m}$.
- At step t, generate a 'candidate' state X_{t+1} from X_t according to Q.
- With probability $\min\left(1, \frac{p(X_{t+1})}{p(X_t)}\right)$, 'accept' the candidate. Else 'reject' the candidate, setting $X_{t+1} = X_t$.

$P(i) \geq P(j)$

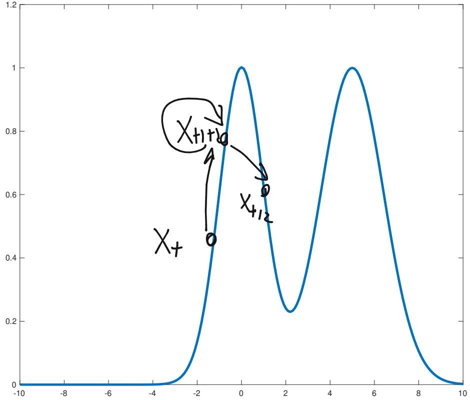
$P_{ij} = Q_{ij} \cdot \frac{P(j)}{P(i)} = Q_{ij} \cdot \frac{\pi(j)}{\pi(i)}$

$P_{ji} = Q_{ji} = Q_{ij}$ symmetry of Q

$\pi(i) \cdot P_{ij} = Q_{ij} \cdot \pi(j) = P_{ji} \cdot \pi(j)$

detailed balance

Metropolis-Hastings Intuition



$\pi(i) P_{ij} \quad = \quad \pi(j) P_{ji}$

Metropolis-Hastings Analysis

Need to check that for the Metropolis-Hastings algorithm, $\pi P = \pi$.

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$$[pP](i) = \underbrace{\sum_j p(j) \cdot Q_{j,i} \cdot \min\left(1, \frac{p(i)}{p(j)}\right)}_{\textcolor{blue}{aceptances}} + \underbrace{p(i) \cdot \sum_j Q_{i,j}\left(1 - \min\left(1, \frac{p(j)}{p(i)}\right)\right)}_{\textcolor{red}{rejections}}$$

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$$= \sum_j Q_{i,j} \cdot \min(p(j), p(i)) + p(i) \cdot \sum_j Q_{i,j} - \sum_j Q_{i,j} \cdot \min(p(i), p(j))$$

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$$= p(i) \cdot \sum_j Q_{i,j}$$

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\begin{aligned}
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&= \sum_j Q_{i,j} \cdot \min\left(p(j), p(i)\right) + p(i) \cdot \sum_j Q_{i,j} - \sum_j Q_{i,j} \cdot \min(p(i), p(j)) \\
&= p(i) \cdot \sum_j Q_{i,j} = p(i).
\end{aligned}
$$

Metropolis-Hastings for the Hard-Core Model

Want to sample an independent set X with probability $\pi(X) = \frac{\lambda^{|X|}}{\sum_{Y \text{ independent}} \lambda^{|Y|}}$.

- Let $p(X) = \lambda^{|X|}$ and let the transition function Q be given by:
  - Pick a random vertex v.
  - If $v \in \mathsf{X}_t$, set $\mathsf{X}_{t+1} = \mathsf{X}_t \setminus \{v\}$
  - If $v \notin \mathsf{X}_t$ and $\mathsf{X}_t \cup \{v\}$ is independent, set $\mathsf{X}_{t+1} = \mathsf{X}_t \cup \{v\}$.
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- Need to accept the transition with probability $\min\left(1, \frac{p(\mathsf{X}_{t+1})}{p(\mathsf{X}_t)}\right)$.

λ if adding vertex

λ^{-1} if removing vertex

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$\lambda < 1$ or $\lambda > 1$

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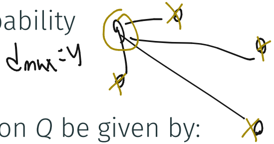

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The key challenge then becomes to analyze the mixing time.

For the related Glauber dynamics, Luby and Vigoda showed that for graphs with maximum degree Δ, when $\lambda < \frac{2}{\Delta - 2}$, the mixing time is $O(n \log n)$. But when $\lambda > \frac{c}{\Delta}$ for large enough constant c, it is NP-hard to approximately sample from the hard-core model.

"show transitions"

MCMC for Approximate Counting

Counting to Sampling Reductions

Often if one can efficiently sample from the distribution $\pi(X) = \frac{p(X)}{\sum_Y p(Y)}$, one can efficiently approximate the normalizing constant $Z = \sum_Y p(Y)$ (often called the partition function).

- If Z is hard to approximate, then this can give a proof that sampling is hard, and thus it is unlikely that any simple MCMC method for sampling from π mixes rapidly.
- This is e.g., how one can show that sampling from the hard-core model is hard when $\lambda = \Omega(1/\Delta)$.

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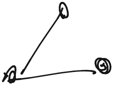
- This is e.g., how one can show that sampling from the hard-core model is hard when $\lambda = \Omega(1/\Delta)$.
- Let's consider the simple case of $\lambda = 1$. I.e., we want to sample a uniformly random independent set.
- In this case, $Z = |S(G)|$, the number of independent sets in G. It is known that approximating $|S(G)|$ even up to a poly(n) factor is NP-Hard.



$|S(G)| \doteq Y$

Counting Independent Sets

How can we count the number of independent sets $|S(G)|$ in a graph, given an oracle for sampling a uniform random independent set?

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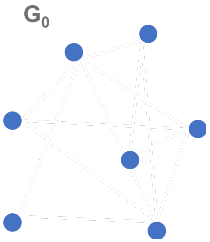

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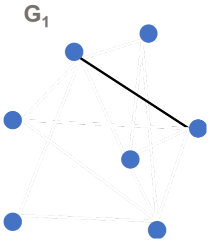

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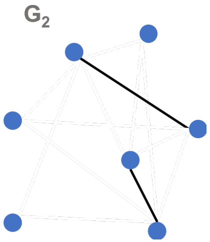

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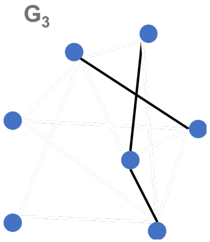

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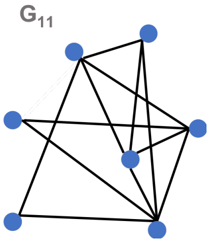

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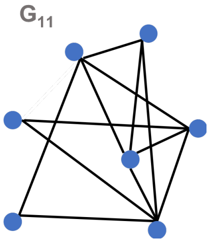

estimate via sampling.

We can write:

$$|S(G)| = \frac{|S(G_m)|}{|S(G_{m-1})|} \cdot \frac{|S(G_{m-1})|}{|S(G_{m-2})|} \cdot \ldots \cdot \frac{|S(G_1)|}{|S(G_0)|} \cdot |S(G_0)|.$$

2^n

Counting Independent Sets

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where $r_i = \frac{|S(G_{m-i+1})|}{|S(G_{m-i})|}$.

Counting Independent Sets

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where $r_i = \frac{|S(G_m)|}{|S(G_{m-i})|}$. If we can estimate each r_i with $\tilde{r}_i$ satisfying

$$\left(1 - \frac{\epsilon}{2m}\right) \cdot r_i \leq \tilde{r}_i \leq \left(1 + \frac{\epsilon}{2m}\right) \cdot r_i,$$

then:

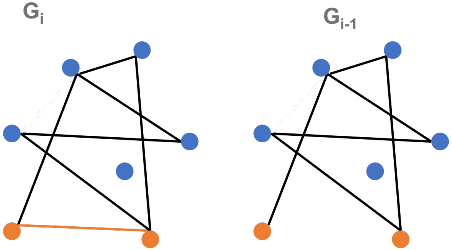
$$(1 - \epsilon) \cdot |S(G)| \leq 2^n \cdot \Pi_{i=1}^{m} \tilde{r}_i \leq (1 + \epsilon) \cdot |S(G)|$$

since $\left(1 + \frac{\epsilon}{2m}\right)^m \leq 1 + \epsilon$ and $\left(1 - \frac{\epsilon}{2m}\right)^m \geq 1 - \epsilon$.

Independent Set Ratios

Consider the ratio $r_i = \frac{|S(G_i)|}{|S(G_{i-1})|}$. Observe that $r_i \leq 1$.

Further, $r_i \geq 1/2$. Let (u, v) be the edge removed from G_i to obtain G_{i-1}. Then each independent set in $S(G_{i-1}) \setminus S(G_i)$, must contain both u and v.



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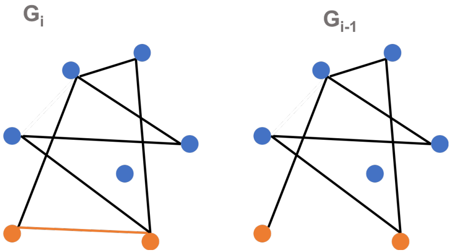

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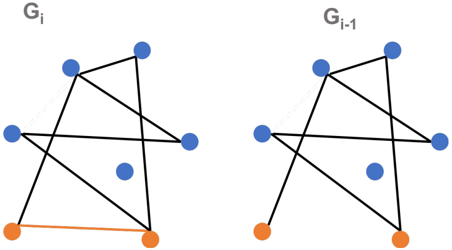

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$$r_i = \frac{|S(G_i)|}{|S(G_{i-1})|} = \frac{|S(G_i)|}{|S(G_i)| + |S(G_{i-1}) \setminus S(G_i)|} \geq \frac{1}{2}.$$

Independent Set Ratios

So Far: We have written $|S(G)| = 2^n \cdot \Pi_{i=1}^m r_i$ where $r_i = \frac{|S(G_i)|}{|S(G_{i-1})|}$. Need to get a $1 \pm \epsilon/m$ estimate to each r_i to get a $1 \pm \epsilon$ estimate to $|S(G)|$.

Independent Set Ratios

So Far: We have written $|S(G)| = 2^n \cdot \Pi_{i=1}^m r_i$ where $r_i = \frac{|S(G_i)|}{|S(G_{i-1})|}$. Need to get a $1 \pm \epsilon/m$ estimate to each r_i to get a $1 \pm \epsilon$ estimate to $|S(G)|$.

Let X be a random variable generated as follows: pick a random independent set from G_{i-1} and let $\mathsf{X} = 1$ if the set is also independent in G_i. Otherwise let $\mathsf{X} = 0$.

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What is $\mathbb{E}[\mathbf{X}]$? $= Pr(X=1) = \frac{|S(G_i)|}{|S(G_{i-1})|} = r_i$

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What is $\mathbb{E}[\mathbf{X}]$?

How many samples of $\mathbf{X}$ do we need to take to obtain a $1 \pm \epsilon/m$ approximation to r_i with high probability?

$\tilde{O}\left(\frac{m^2}{\epsilon^2}\right)$

Counting Independent Sets

Upshot: For a graph G with m edges, making $\tilde{O}(m^2/\epsilon^2)$ calls to a uniform random independent set sampler on G or its subgraphs suffices to approximate the number of independent sets in G up to $1 \pm \epsilon$ relative error.

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- So a polynomial time algorithm for uniform random independent set sampling, would lead to a polynomial time algorithm for counting independent sets, and hence the collapse of NP to P.
- Observe that near-uniform sampling (as would be obtained e.g., with an MCMC method) would also suffice.