Monte Carlo Method

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Outline

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If a solution to a self-reducible combinatorial problem can be sampled, we can construct a randomized algorithm which counts the number of solutions.

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A sampling algorithm is a fully polynomial almost uniform sample (*FPAUS*) for a problem if, given an input x and a parameter $\varepsilon > 0$, it generates an ε - uniform sample of $\Omega(x)$ and runs in time that is polynomial in $\ln \varepsilon^{-1}$ and the size of the input x.

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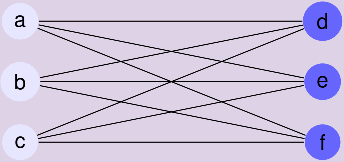

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Input : Graph $G = (V, E)$ and parameter ε.

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Output : ε-uniform sample of the independent sets.

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Input : Graph $G = (V, E)$ and parameter ε.
Sample space : All independent sets in G.
Output : ε-uniform sample of the independent sets.
Goal : To show that, given an FPAUS for independent sets, we can construct an FPRAS for counting the number of independent sets.

Example

Continued

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Input graph G has m edges.

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E_i be the set of the first i edges in E.

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The number of independent sets in G can be expressed as,

$$|\Omega(G)| = \frac{|\Omega(G_m)|}{|\Omega(G_{m-1})|} \times \frac{|\Omega(G_{m-1})|}{|\Omega(G_{m-2})|} \times \frac{|\Omega(G_{m-2})|}{|\Omega(G_{m-3})|} \times \cdots \times \frac{|\Omega(G_1)|}{|\Omega(G_0)|} \times |\Omega(G_0)|.$$

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To have an (ε, δ)-approximation, we want $P(|R - 1| \leq \varepsilon) \geq 1 - \delta$.

Lemmas

Lemma

Suppose that for all i, $1 \leq i \leq m$, $\tilde{r}_i$ is an $(\frac{\varepsilon}{2 \cdot m}, \frac{\delta}{m})$-approximation for r_i. Then,

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Proof

For each $1 \leq i \leq m$, we have

$$\begin{aligned} P(|\tilde{r}_i - r_i| \leq \frac{\varepsilon}{2 \cdot m} \cdot r_i) &\geq 1 - \frac{\delta}{m} \\ P(|\tilde{r}_i - r_i| > \frac{\varepsilon}{2 \cdot m} \cdot r_i) &< \frac{\delta}{m} \end{aligned}$$

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By union bound, the probability that $|\tilde{r}_i - r_i| > (\frac{\varepsilon}{2 \cdot m}) \cdot r_i$ for any i is at most δ;
Therefore $|\tilde{r}_i - r_i| \leq (\frac{\varepsilon}{2 \cdot m} \cdot r_i)$ for all i with probability at least $1 - \delta$. Equivalently,

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$$1 - \frac{\varepsilon}{2 \cdot m} \leq \frac{\tilde{r}_i}{r_i} \leq 1 + \frac{\varepsilon}{2 \cdot m}$$

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Notes

We need a method for obtaining an $(\frac{\varepsilon}{2\cdot m}, \frac{\delta}{m})$- approximation for the r_i.
We estimate each of these ratios by a Monte Carlo algorithm that uses *FPAUS* for sampling independent sets.

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To estimate r_i, we sample independent sets in G_{i-1} and compute the fraction of these sets that are also independent sets in G_i, as shown in the following algorithm.

Algorithm

Estimating r_i:

Input: Graphs $G_{i-1} = (V, E_{i-1})$ and $G_i = (V, E_i)$.
Output: $\tilde{r}_i$ = an approximation of r_i.

1: $X \leftarrow 0$
2: **repeat**
3: Generate an $(\frac{\varepsilon}{6 \cdot m})-$ uniform sample from $\Omega(G_{i-1})$.
4: If the sample is an independent set in G_i, let $X \leftarrow X + 1$.
5: **until** $M = \lceil 1296 m^2 \varepsilon^{-2} \ln(\frac{2 \cdot m}{\delta}) \rceil$ independent trials
6: **return** $\tilde{r}_i \leftarrow \frac{X}{M}$

Algorithm 2.1: Estimating r_i

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associate each $I \in \Omega(G_{i-1}) \setminus \Omega(G_i)$ with an independent set $I \setminus v \in \Omega(G_i)$.
We have,

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

Lemmas

continued

Consider M samples and let X_k be

$$X_k = \begin{cases} 1 & \text{if the } k^{\text{th}} \text{ sample is in } \Omega(G_i) \\ 0 & \text{otherwise} \end{cases}$$

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$$|P(X_k = 1) - \frac{|\Omega(G_i)|}{|\Omega(G_{i-1})|}| \leq \frac{\varepsilon}{6 \cdot m}.$$

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Since X_k are indicator random variables and further by linearity of expectations, we get

$$|\mathbf{E}[\tilde{r}_i] - r_i| \quad = \quad |\mathbf{E}[\frac{\sum_{i=1}^{M} X_k}{M}] - \frac{|\Omega(G_i)|}{|\Omega(G_{i-1})|}| \leq \frac{\varepsilon}{6 \cdot m}.$$

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Lemma is completed by combining

(a) $\mathbf{E}[\tilde{r}_i]$ is close to r_i and

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Using the above and $r_i \geq 1/2$ gives the desired $(\frac{\varepsilon}{2 \cdot m}, \frac{\delta}{m})$- approximation.

Theorems

Theorem

Given a fully polynomial almost uniform sampler (*FPAUS*) for independent sets in any graph, we can construct a fully polynomial randomized approximation scheme (*FPRAS*) for the number of independent sets in a graph G.

Theorem

Given a fully polynomial almost uniform sampler (*FPAUS*) for independent sets in any graph with maximum degree at most Δ, we can construct a fully polynomial randomized approximation scheme (*FPRAS*) for the number of independent sets in a graph G with maximum degree at most Δ.

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Where MCMC is used

(i) Data Mining and Machine Learning
(ii) Bayesian methods
(iii) Biological and generic research

Recall Markov chain

Questions

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(iv) Stationary distribution? A stationary distribution of a Markov chain is a probability distribution $\bar{\pi}$ such that $\bar{\pi} = \bar{\pi} \cdot P$

Recall Markov chain continued

Theorem (for stationary distribution)

Consider a finite, irreducible, and ergodic Markov chain with transition matrix P. If there are nonnegative numbers $\bar{\pi} = (\pi_0, ...\pi_n)$ such that $\sum_{i=0}^{n} \pi_i = 1$ and if, for any pair of states i, j,

$$\pi_i \cdot P_{i,j} = \pi_j \cdot P_{j,i},$$

then $\bar{\pi}_i$ is the stationary distribution corresponding to P.

Recall Markov chain continued

Theorem (for stationary distribution)

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Theorem

A random walk on G converges to a stationary distribution $\bar{\pi}$, where

$$\pi_v = \frac{d(v)}{2 \cdot |E|}.$$

In a stationary distribution of a random walk, the probability of a vertex is proportional to the degree of the vertex.

MCMC Continued

Basic Idea

Define an ergodic Markov chain whose set of states is the sample space and whose stationary distribution is the required sampling distribution.

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Similarly starting from X_r, $X_{2.r}$ can be used as a sample and so on.
Therefore the sequence of states $X_r, X_{2.r}, X_{3.r}, \ldots$ can be used as the almost independent samples from the stationary distribution of the Markov chain.

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If this chain is irreducible and aperiodic, then the stationary distribution is the uniform distribution.

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Outline

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Assume we have designed an irreducible state space for a Markov chain.
We want to construct Markov chain on this state space with a stationary distribution, $\pi_x = \frac{b(x)}{B}$, $\forall x \in \Omega$ we have $b(x) > 0$ such that $B = \sum_{x \in \Omega} b(x)$ is finite.

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Then, if this chain is irreducible and aperiodic, the stationary distribution is given by the probabilities π_x.

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Choose a vertex v to add or delete with probability $\frac{1}{M}$; here $M = |V|$.

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The transition probability $P_{x,y} = \frac{1}{M} \cdot min(1, \frac{\pi_y}{\pi_x})$, so Lemma applies.

Metropolis Algorithm

Notes

We dint need to know $B = \sum_x \lambda^{|I_x|}$.
Graphs with n vertices can have exponentially many independent sets calculating whose sum would be expensive task.
Markov chain here gives the stationary distribution by using only the ratios $\frac{\pi_y}{\pi_x}$.