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### Approximate Counting

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#### Introduction

### Example: Estimating $\pi$

Chose a point, (X, Y), in a 2 × 2 square centered at (0,0).
Or equiv chose Y and X independently from [-1,1].

• 
$$Z = \begin{cases} 1 & \text{if}(X, Y) \in \text{Unit Circle} \\ 0 & otherwise \end{cases}$$

- $Pr(Z = 1) = \frac{\pi}{4}$  the ratio of the area of the cicle to the area of the square.
- We run *m* times and let  $W = \sum_{i=1}^{m} Z_i$ .
- $\mathbb{E}[W] = \frac{m\pi}{4}$  and W' = (4/m)W is a natural estimate for  $\pi$ .
- By Chernoff bound (Pr(|X μ| ≥ δμ) ≤ 2e<sup>μδ<sup>2</sup>/3</sup>, where X is the sum of independent poisson trials) we have:
   Pr(|W' π| ≥ επ) ≤ 2e<sup>-mπε<sup>2</sup>/12</sup>

The Markov Chain Monte Carlo Method

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#### Introduction

## $(\varepsilon, \delta)$ -approximation and FPRAS

#### Definition (( $\varepsilon, \delta$ )-approximation)

A randomized algorithm gives an  $(\varepsilon, \delta)$ -approximation for the value *V* if the output *X* satisfies:

$$Pr(|X - V| \le \varepsilon V) \ge 1 - \delta.$$

Therefore if we choose  $m \ge \frac{12 \ln(2/\delta)}{\pi \varepsilon^2}$  we have an  $(\varepsilon, \delta)$ -approximation for  $\pi$ .

#### Definition

A fully polynomial randomized approximation scheme for a problem is a randomized algorithm for which, given an input x and any parameters  $0 < \varepsilon, \delta < 1$ , the algorithm outputs an  $(\varepsilon, \delta)$ -approximation to V(x) in time polynomial in  $1/\varepsilon$ ,  $\ln \delta^{-1}$  and the size of the input x.

The Markov Chain Monte Carlo Method

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Introduction

### Outline of the Monte Carlo Method

#### Obtain an efficient approximation for a value V:

Find an efficient Process to generate a sequence of of independent and identically distributed random samples with  $\mathbb{E}[X_i] = V$ .

Get enough samples for an  $(\varepsilon, \delta)$ -approximation for *V*.

# The nontrivial task here is to Generate a good sequence of samples.

The Monte Carlo method is also called Monte Carlo Simulation.

## A little about counting problems

- In counting problems we are interested in finding the number of different solutions for the input.
- For example in #SAT we are interested in counting the number of satisfying assignments of a given boolean formula in conjunctive normal form.
- The class of counting problems that can be solved within poly-time is FP

The output is a number and not a yes/no answer as in decision problems

 The class that contains the problems of counting the solutions of NP problems is called #P.

## A little about counting problems (cont.)

- #P = {f | f(x) = acc<sub>M</sub>(x)}, where M is a NPTM and acc<sub>M</sub>(x) = number of accepting paths of M on input x.
- With an a-la-cook proof we can get that #SAT is a complete problem for #P.
- It is interesting the fact that counting versions of problems in *P* may also be complete for #P.
  - examples: #BIPMATCHINGS, #DNFSAT, #MONSAT, #IS, #BIS.
- Note that these hard to count easy to decide problems are #P complete under the poly-time Turing reduction and #P is not closed under poly-time Turing reduction.
- On the other hand #P is closed under poly-time many one reduction (parsimonious or karp).

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DNFSAT Counting

## A little about counting problems (concl.)

- Furthermore there are three degrees of approximability within problems of #P [DGGJ'00]:
  - Solvable by an *FPRAS*: #PM, #DNFSAT, ...
  - AP-interreducible with #SAT: #SAT, #IS, #IS<sub>ldeg(25)</sub> ...
  - An Intermediate Class (AP-Interreducible with #BIS)

Note that if the counting versions of NP complete problems have an FPRAS this would imply an unexpected class collision (NP = RP).

## **#DNFSAT:** A first approach

• Given a **#DNFSAT** formula *F* consider the following algorithm:

- For k = 1 to m do:
  - a Generate a random assignment for the *n* variables, chosen uniformly at random from all 2<sup>*n*</sup> possible assignments
  - b If the random assignment satisfies the formula: X := X + 1

3 Return  $(X/m)2^n$ .

- If  $X = \sum_{i=1}^{m} X_i$ , where  $X_i$  independent random variables that take value 1 with probability c(F)/n
- By linearity of expectations:  $\mathbb{E}[Y] = \frac{\mathbb{E}[X]2^n}{m} = c(F)$ , where c(F) = # sat assingns.

The Markov Chain Monte Carlo Method

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**DNFSAT** Counting

### A first approach (concl.)

• The previous approach gives an  $(\varepsilon, \delta)$ -approximation of c(F) when  $m \ge \frac{3 \cdot 2^n \ln(2/d)}{\varepsilon^2 c(F)}$ 

## A first approach (concl.)

- The previous approach gives an  $(\varepsilon, \delta)$ -approximation of c(F) when  $m \ge \frac{3 \cdot 2^n \ln(2/d)}{\varepsilon^2 c(F)}$
- The above algorithm is polynomial to the size of the input (n) only if c(F) ≥ 2<sup>n</sup>/poly(n)
- We have no guarantee of how dense c(F) is in our sample space
- If c(f) is polynomial in n then with high probability we must sample an exponential number of assignments before finding the fist satisfying one.

#### Fixing the sample space

- A sat assignment of *F* = C<sub>1</sub> ∨ C<sub>2</sub>...C<sub>t</sub> needs to satisfy at least one of the clauses.
- If clause C<sub>i</sub> has I<sub>i</sub> litterals there are exactly 2<sup>n-l<sub>i</sub></sup> sat assigns.
- If *SC<sub>i</sub>* is the set of assigns that sat *C<sub>i</sub>* we will use as sample space the following:

$$U = \{(i, a) \mid 1 \leq i \leq t \quad \& \quad a \in SC_i\}.$$

- $|U| = \sum_{i=1}^{t} |SC_i|$  and we want to compute  $c(F) = \left|\bigcup_{i=1}^{t} SC_i\right|$ .
- An assignment can satisfy more than one clause, thus we need to define a subset S ⊆ U with size c(F).

## The Algorithm

• We provide the following algorithm for sampling

$$\bigcirc X := 0$$

- 2 For *k* := 1 to *m* do:
  - a With probability  $|SC_i|/|U|$  choose, uniformly at random, an assignment  $a \in SC_i$
  - b If a is not in any  $SC_j$ , j < i, then X := X + 1.
- 3 Return (X/m)|U|
- The above algorithm in order to estimate c(F) uses
  - $\boldsymbol{S} = \{(i, \boldsymbol{a}) \mid 1 \leq i \leq t, \boldsymbol{a} \in \boldsymbol{SC}_i, \boldsymbol{a} \notin \boldsymbol{SC}_j \quad \text{for} \quad j < i\}.$ 
    - That is for each sat assign we get exactly one pair, the one with the smalest clause index number.
- Then we estimate the ratio |S|/|U| by sampling uniformly at random from *U*.

### FPRAS for **#DNFSAT**

- How to uniformly sample from *U*:
  - We first choose the first coordinate *i*.
  - The *i*-th clause has  $|SC_i|$  sat assigns, therefore we should chose *i* with probability proportional to  $|SC_i|$ , that is we chose *i* with probability  $|SC_i|/|U|$ .
  - Then we chose a sat assign uniformly at random from *SC<sub>i</sub>*, that is we chose the value "T" or "F" independently and uniformly at random for each variable not in clause *i*.
- Pr((i, a) is chosen ) = Pr(a is chosen | i is chosen)=  $\frac{|SC_i|}{|U|} \cdot \frac{1}{|SC_i|} = \frac{1}{|U|}$ , which gives a uniform distribution.
- This algorithm is an FPRAS when  $m = \lceil (3t/\varepsilon^2) \ln(2/\delta) \rceil$ .

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DNFSAT Counting

### FPRAS for #DNFSAT (concl.)

This algorithm is an FPRAS when  $m = \lceil (3t/\varepsilon^2) \ln(2/\delta) \rceil$ .

- A sat assign of F sats at most t clauses, therefore there are at most t elements (i, a) in U, corresponding to each C<sub>i</sub>
- therefore  $\frac{|S|}{|U|} \ge \frac{1}{t}$ , that is the probability that each random chosen element belongs to *S* is at least 1/t. ( $\mathbb{E}[X] \ge 1/t$ )

• 
$$Pr(|\mathbb{E}[Y] - |S|| \ge \varepsilon \mathbb{E}[Y]) =$$
  
 $Pr(|\mathbb{E}[X] - |S|m| \ge \varepsilon \mathbb{E}[X]m) \le$   
 $2e^{-\varepsilon^2 \mathbb{E}[X]m/3} \le \delta$ 

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#### Introduction

#### Markov Chains Reminder

- MC is a stohastic process that has states and transition probabilities.
- The transition probabilities are memoryless, i.e. they depend only on the current state of the MC.
- An ergodic (irreducible, finite and aperiodic) Markov Chain converges to a unique stationary distribution π.
  - That is the probability of a state in the MC is given by  $\pi$ , and it is independent from the initial state.

#### Introduction

### Overview of the MCMC method

- Define an ergodic Markov Chain with states the elements of the Sample Space.
- This MC must converge to the required Sampling Distribution.
- From any starting state X<sub>0</sub>, and after a sufficient number of steps *r* the distribution of X<sub>r</sub> will be close to the stationary.
- We use as almost independent samples *X<sub>r</sub>*, *X<sub>2r</sub>*, *X<sub>3r</sub>*....
- The efficiency of MCMC method depends on:
  - How large *r* must be to have a good samples.
  - How fast (computationally) can we traverse between the states of the MC.

From Sampling to Counting

## Variation Distance and Approximate Samplers

#### Definition (Variation Distance)

The variation distance between two probability distributions  $\pi$  and  $\pi'$  on a countable state space *S* is given by:  $\|\pi - \pi'\| = \frac{1}{2} \sum_{x \in S} |\pi(x) - \pi'(x)|.$ 

• 
$$\|\pi - \pi'\| = \max_{A \subseteq S} |\pi(A) - \pi'(A)|$$

#### **Definition (FPAUS)**

An almost uniform sampler is a randomized algorithm that takes as input *x* and a tolerance  $\delta$ , and produces a random variable  $Z \in \Omega(x)$ , such that the probability distribution of *Z* is within variation distance  $\varepsilon$ of the uniform distribution on  $\Omega(x)$ . An almost uniform sampler is said to be fully polynomial if it runs in poly-time in |x| and  $\ln \delta^{-1}$ .

Notice that the above definition can be generalized for any desired distribution.

The Markov Chain Monte Carlo Method

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From Sampling to Counting

### An Example: Proper Colorings of a Graph

#### Theorem

Suppose we have an AUS for k-colorings of a graph, which works for graphs G with max degree  $\Delta < k$ ; and suppose that the sampler has time complexity  $T(n, \delta)$  (n is the number of vertices in G). Then we may construct a ( $\varepsilon$ ,  $\delta$ )-approximation for the number of k-colorings of a graph, which works for graphs with max degree bounded by  $\Delta$ , and which has time complexity  $\mathcal{O}(\frac{m^2}{\varepsilon^2}T(n,\frac{\varepsilon}{6m}))$ .

The idea of the proof will be presented on the whiteboard.

#### Markov Chains and Mixing Time

## Markov Chain with Uniform distribution

- We need a MC with uniform stationary distribution.
- We perform a random walk in the graph of the state space.
- We add self loops to break the periodicity of MC.
- Lemma:

For a finite space  $\Omega$  and neigborhood structure  $\{N(x) \mid x \in \Omega\}$  let  $N = \max_{x \in \Omega} |N(x)|$ . Let  $M \ge N$ . If the following MC is irreducible, aperiodic then the sationary distribution is the uniform distribution.

$$P_{x,y} = \begin{cases} 1/M & \text{if } x \neq y \text{ and } y \in N(x), \\ 0 & \text{if } x \neq y \text{ and } y \notin N(x), \\ 1 - N(x)/M & \text{if } x = y. \end{cases}$$

Markov Chains and Mixing Time

### Markov Chain for the k-colorings

- For our example we will use the following Markov Chain: At each step choose a vertex v u.a.r. and a color c u.a.r. Recolor v with c if the new coloring is proper, otherwise the state of the chain remains unchainged
- This chain obviously satisfies the requirements of the previous lemma.
- We will show that the above MC is "rapidly mixing", that is the *t*-step distribution closely approaches to the stationary distribution in polynomial time (of *n*), provided k ≤ 2Δ + 1.

Markov Chains and Mixing Time

## **Mixing Time**

#### Definition

Let  $\pi$  be the stationary disrtibution of a Markov Chain with state space *S*. Let  $p_x^t$  be the distribution of the state of the chain starting at *x* after *t* steps. We define:  $\Delta_x(t) = \|p_x^t - \pi\|.$ 

#### Definition (Mixing Time)

We define  $\tau_x(\varepsilon) = \min\{t \mid \Delta_x(t) \le \varepsilon\}$  and  $\tau(\varepsilon) = \max_{x \in S} \tau_x(\varepsilon)$ . That is  $\tau_x(\varepsilon)$  is the first step *t* at which the variation distance between  $p_x^t$  and the stationary distribution is less than  $\varepsilon$ , and  $\tau(\varepsilon)$  is the maximum of these values over all states *x*.

A chain is called rapidly mixing if  $\tau(\varepsilon)$  is polynomial in  $1/\varepsilon$  and the size of the problem.

Coupling of Markov Chains

#### The main idea

- In order to show that a chain is rapidly mixing consider the following.
- We have two copies of the same Markov Chain one of them already in the sationary distribution.
- The other starts at a state x.
- We then prove that after a short period of time they reach the same state.
- Additionally we have defined the two chains properly so that the remain in the same state right after.

#### Coupling of Markov Chains

## Coupling

#### Definition (MC coupling)

A coupling of a Markov chain  $M_t$  with a state space S is a Markov chain  $Z_t = (X_t, Y_t)$  on the state space  $S \times S$  such that:

$$Pr(X_{t+1} = x' \mid Z_t = (x, y)) = Pr(M_{t+1} = x' \mid M_t = x);$$
  

$$Pr(X_{t+1} = y' \mid Z_t = (x, y)) = Pr(M_{t+1} = y' \mid M_t = y).$$

That is, a coupling consists of two copies of the MC M running simultaneously. They are not necessarily in the same state of make the same move, instead each copy behaves exactly like the original chain.

We will use couplings that:

- bring the two copies to the same state
- keep them in the same state by having the two chains make identical moves once they are in the same state.

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Coupling of Markov Chains

#### **Coupling Lemma**

#### **Coupling Lemma**

Let  $Z_t = (X_t, Y_t)$  be a coupling for a Markov Chain *M*. Suppose that there exists a *T* such that, for every  $x, y \in S$ ,  $Pr(X_T \neq Y_T \mid X_0 = x, Y_0 = y) \leq \varepsilon$ Then  $\tau(\varepsilon) \leq T$ .

That is, for any initial state, the variation distance between the distribution of the state of the chain after T steps and the stationary distribution is at most T.

Proof on board.

#### Coupling of Markov Chains

## FPAUS for k-colorings (I)

- Consider the case of k-colorings where  $k > 2\Delta + 1$
- We remind the MC on the colorings of G: At each step chose a vertex v u.a.r. and a color c u.a.r. Recolor v with c if the new coloring is proper, otherwise let the state unhanged.
- We will define a coupling of this MC.
- Let  $D_t$  be the set of vertices that have different colors in the two chains of the coupling at time *t* with  $|D_t| = d_t$ .
- Let *A<sub>t</sub>* be the set of vertices that have the same color in the two chains at time *t*.
- Define d'(v) to be the neigbours of v in  $D_t$  if  $v \in A_t$ .
- Similarly d'(w) the neigbours of w in  $A_t$  if  $w \in D_t$ .

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#### Coupling of Markov Chains

## FPAUS for k-colorings (II)

- Note that  $\sum_{v \in A_t} d'(v) = \sum_{w \in D_t} d'(w) = m'$ .
- Coupling: If an vertex v ∈ Dt is chosen to be recolored, we chose the same color for both chains.
- The vertex *v* will have the same color in both chains whenever the color chosen is different from any color on any of the neigbors of *v* in both copies of the MC.
- There are  $k 2\Delta + d'(v)$  such colors.
- The probability that  $d_{t+1} = d_t 1$  when  $d_t > 0$  is at least:  $\frac{1}{n} \sum_{v \in D_t} \frac{k - 2\Delta + d'(v)}{k} = \frac{1}{kn} ((k - 2\Delta)d_t + m').$

Coupling of Markov Chains

## FPAUS for k-colorings (III)

- Coupling: If a vertex v ∈ A<sub>t</sub> is chosen to be recolored we use the following:
- If the two vertices have one neighbour with different colors wlog assume v has color 1, and the neigbours have colors 2,3. We recolor v with 3 in the first copy and 2 in the second copy. (dt doesn't increase)
- General case, id there are d'(v) differently colored vertices around v we can couple the colors so that at most d'(v) color choices cause d<sub>t</sub> to increase. (explain)
- the probability that  $d_{t-1} = d_t + 1$  is at most:

$$\frac{1}{n}\sum_{v\in A_t}\frac{d'(v)}{k}=\frac{m'}{kn}.$$

#### • After some calculations (board) we prove that: $\tau(\varepsilon) \leq \frac{n(k-\Delta)}{k-2\Delta} \ln(\frac{n}{\varepsilon})$

Other Mixing Time Bounding Methods

## Path Coupling

- We will explain the intuition of Path coupling with the problem #IS (it works for max deg  $\leq$  4).
- We start with a coupling for pairs of states thad differ in just one vertex.
- Then we extend this to a general coupling over all pairs of states.
- This technique is powerfull because it is often much easier to analyze the situation where the two states differ in a small way, than to analyze all possible ways of states.
- The extention of the coupling is a chain of states Z<sub>0</sub>...Z<sub>dt</sub> where Z<sub>0</sub> = X<sub>t</sub> and Y<sub>t</sub> = Z<sub>dt</sub>, an each successive Z<sub>i</sub> is obtained from Z<sub>i-1</sub> by either removing a vertex from X<sub>t</sub> \ Y<sub>t</sub> or adding a vertex from Y<sub>t</sub> \ X<sub>t</sub>.
- The previous can be done for example by first removing all vertices in X<sub>t</sub> \ Y<sub>t</sub> one by one and then add all the vertices in Y<sub>t</sub> \ X<sub>t</sub> one by one.

The Markov Chain Monte Carlo Method

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Other Mixing Time Bounding Methods

### Canonical Paths, CFTP

#### Canonical Paths

- View the MC as an undirected gaph with vertex set Ω and edge set E = {{x, y} ∈ Ω<sup>2</sup> | P(x, y) > 0}.
- For each ordered pair (x, y) we specify a canonical path γ<sub>xy</sub> in the graph.
- We choose a set of paths that avoid teh creation of edges that carry a heavy burden of paths
- intuitively we might expect a MC to be rapidly mixing if it contains no "bottlenecks".
- Coupling from the Past
  - We use "algorithmic coupling" to obtain sample from the exact stationary distribution.

#### Permanent

## **Definition and History**

• The permanent for a  $n \times n$  zero one matrix is deifined by:

$$\operatorname{per}(A) = \sum_{\pi} \prod_{i=1}^{n} A_{1,\pi(i)}$$

where the sum is over all permutations  $\pi$  of  $\{1, 2, ..., n\}$ .

- The best deterministic algorithm runs in time  $\mathcal{O}(n2^n)$
- Although the determinant can be computed in poly time by gaussian elimination.
- It is equivalent to #BIPMATCHINGS, if A is the adjacency matrix.
- Valiant has shown that it is #P-complete.

#### Permanent

### FPRAS for the Permanent

- An FPRAS was given by Jerrum, Sinclair and Vigoda '02.
- It is based in a Markov Chain monte carlo method.
- The sample space of the MC consists of all perfect and near-perfect Matchings (matchings with two uncovered vertices).
- The problem is that near-perfect mathcings may outnumber the pm's by more than a polynomial factor.
- Solution: a weighting of the near perfect matchings in the stationary distribution so as to take acount the position of the holes (not matched vertices).
- Each hole pattern has equal aggregated weigt so the PM's are not dominated too much
- The mixing time of the chain is bounded by Canonical Paths Method (ロ) (同) (三) (三) (三) (○) (○)

#### Permanent

## An alternative estimator (Simple Approach)

- The Laplace's expantion formula for the Permanent:  $per(A) = \sum_{j=1}^{n} a_{1j} per(A_{1j})$
- The algorithm is the following:

If n = 0 then  $X_A = 1$ .  $W := \{j \mid a_{1j} = 1\}$ . If  $W = \emptyset$  then  $X_A = 0$ . else chose J u.a.r. from W $X_A = |W|X_{A_{1j}}$ .

- For this estimator it holds that:
  - $$\begin{split} \mathbb{E}[X_A] &= \operatorname{per}(A) \\ \mathbb{E}[X_A^2] &= \operatorname{per}^2(A)n!. \ \text{(equality for the upper triangular)} \end{split}$$
- The important result here is that for any function  $\omega(n)$

$$Pr_{A_n}\left(rac{\mathbb{E}[X_A^2]}{(\mathbb{E}[X_A])^2} > n\omega(n)
ight) o 0$$

That is the number of trials is bounded by  $O(n\omega(n)/\varepsilon^2)$  with high probability.