Randomized Algorithms

The Monte Carlo Method

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Outline

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Introduction

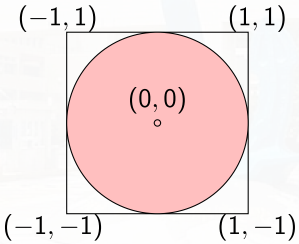
- The Monte Carlo method: estimating values through sampling and simulation.
- Widely used in almost all areas of physical sciences and engineering.

Introduction (example)

- As a motivating example, consider the following approach for estimating the constant π.

Estimating π

- Let (X, Y) be a point chosen uniformly at random in a 2×2 square centered at the origin $(0, 0)$.



- demo code on Colab

Estimating π (indicator variable)

- Define the random variable

$$Z = \begin{cases} 1, & \text{if } \sqrt{X^2 + Y^2} \leq 1, \\ 0, & \text{otherwise.} \end{cases}$$

- The probability that $Z = 1$ is the ratio

$$\Pr[Z = 1] = \frac{\text{area of unit circle}}{\text{area of square}} = \frac{\pi}{4}.$$

Estimating π (sampling)

- Run this experiment m times, and let Z_i be the value of Z in the i-th run.
- Define
$$W = \sum_{i=1}^{m} Z_i.$$
- Then
$$\mathbb{E}[W] = \sum_{i=1}^{m} \mathbb{E}[Z_i] = m \cdot \frac{\pi}{4}.$$
- Hence
$$W' = \frac{4}{m} W$$
is a natural estimate for π.

Estimating π (Chernoff bound)

- Using Chernoff bounds on W, we can bound the error of W'.
- For $0 < \varepsilon < 1$,

$$\begin{aligned}\Pr\left[|W' - \pi| \geq \varepsilon\pi\right] &= \Pr[|W - m\pi/4| \geq \varepsilon\, m\pi/4] \\ &= \Pr[|W - \mathbb{E}[W]| \geq \varepsilon\mathbb{E}[W]] \\ &\leq 2e^{-m\pi\varepsilon^2/12}.\end{aligned}$$

- Thus, with sufficiently many samples, we can obtain an arbitrarily tight approximation of π with high probability.

(ϵ, Δ)-approximation randomized algorithm

Definition.

- A randomized algorithm gives an (ε, Δ)-*approximation* for a value V if its output X satisfies

$$\Pr\left[\, |X - V| \le \varepsilon V \,\right] \ \ge\ 1 - \Delta.$$

- Our method for estimating π gives an (ε, Δ)-approximation as long as $\varepsilon < 1$ and m is large enough.
- From the Chernoff bound:

$$2e^{-m\pi\varepsilon^2/12} \le \Delta \quad \Longrightarrow \quad m \ \ge\ \frac{12}{\pi\varepsilon^2} \ln \frac{2}{\Delta}.$$

- Further reading: Probably Approximately Correct (PAC)

A general sampling theorem

Theorem 1.

Let $X_1, \ldots, X_m$ be independent and identically distributed indicator random variables with $\mu = \mathbb{E}[X_i]$. If

$$m \geq \frac{3 \ln(2/\Delta)}{\varepsilon^2 \mu},$$

then

$$\Pr\left[\left|\frac{1}{m}\sum_{i=1}^{m} X_i - \mu\right| \geq \varepsilon\mu\right] \leq \Delta.$$

Thus, m samples provide an (ε, Δ)-approximation for μ.

Approximation schemes

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- It is therefore unlikely that such exact algorithms exist.
- Instead, we study approximation algorithms and approximation schemes:
    - Polynomial-time approximation schemes (PTAS)
    - Fully polynomial-time approximation schemes (FPTAS)
    - Polynomial randomized approximation schemes (PRAS)
    - Fully polynomial randomized approximation schemes (FPRAS)

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  - Polynomial randomized approximation schemes (PRAS)
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- In this lecture, we will focus on PRAS and FPRAS.

Counting problems

- We focus on counting problems that map inputs x to values $V(x)$.
- Example:
  - Given a graph, we may want an approximation to the *number* of independent sets in the graph.
  - Given a Boolean formula in Disjunctive Normal Form (DNF), which is a disjunction of conjunctions of literals, count the *number* of satisfying assignments.

PRAS

Definition (PRAS)

- A *polynomial randomized approximation scheme* (PRAS) for a problem is a randomized algorithm such that, given input x and parameters ε, Δ with $0 < \varepsilon, \Delta < 1$, it outputs an (ε, Δ)-approximation to $V(x)$ in time poly$(|x|)$.

FPRAS

Definition (FPRAS)

- A *fully polynomial randomized approximation scheme* (FPRAS) for a problem is a randomized algorithm such that, given input x and parameters ε, Δ with $0 < \varepsilon, \Delta < 1$, it outputs an (ε, Δ)-approximation to $V(x)$ in time

$$\text{poly}\big(|x|, 1/\varepsilon, \ln(1/\Delta)\big).$$

Outline

The DNF counting problem

- We consider the problem of counting the number of satisfying assignments of a Boolean formula in *disjunctive normal form* (DNF).

Definition

- A DNF formula is a disjunction of clauses

$$F = C_1 \vee C_2 \vee \cdots \vee C_t, \ t \in \mathbb{N}$$

  where each clause is a conjunction of literals.
- Example:

$$(X_1 \wedge \neg X_2 \wedge X_3) \vee (X_2 \wedge X_4) \vee (X_1 \wedge X_3 \wedge \neg X_4).$$

#P and #P-completeness

Class #P

A problem is in the class #P if there is a polynomial-time nondeterministic Turing machine (algorithm) such that, for any input I, the number of accepting computations equals the number of solutions associated with I.

- Clearly, a #P problem is at least as hard as the corresponding NP decision problem.

#P-complete

A problem is #P-complete if it is in #P and every problem in #P can be reduced to it in polynomial time.

- Examples:
  - Counting Hamiltonian cycles in a graph.
  - Counting perfect matchings in a bipartite graph.

Example: From CNF to DNF via Negation

- CNF formula H with three clauses:

$$H = (x_1 \vee \neg x_2 \vee x_3) \wedge (\neg x_1 \vee x_2) \wedge (\neg x_2 \vee \neg x_3).$$

- Negate H and apply De Morgan's laws:

$$\begin{aligned} \neg H &= \neg\left[(x_1 \vee \neg x_2 \vee x_3) \wedge (\neg x_1 \vee x_2) \wedge (\neg x_2 \vee \neg x_3)\right] \\ &= \neg(x_1 \vee \neg x_2 \vee x_3) \vee \neg(\neg x_1 \vee x_2) \vee \neg(\neg x_2 \vee \neg x_3) \\ &= (\neg x_1 \wedge x_2 \wedge \neg x_3) \vee (x_1 \wedge \neg x_2) \vee (x_2 \wedge x_3). \end{aligned}$$

- $\neg H$ is in DNF (a disjunction of conjunctions of literals). Each CNF clause of H becomes one conjunction in $\neg H$.

Hardness of DNF counting

- Counting the number of satisfying assignments of a DNF formula is #P-complete.
- Sketch:
  - Given any CNF formula H, apply De Morgan's laws to obtain a DNF formula $\bar{H}$ (the negation of H) with the same number of variables and clauses.

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- Hence DNF counting is at least as hard as SAT (NP-hard).
  - #satisfying assignment of $H = 2^n -$ #satisfying assignment of $\bar{H}$.
  - Hence we can obtain a polynomial time reduction from #SAT to DNF-counting, where #SAT is known to be #P-complete.

Why approximation for DNF counting?

- It is unlikely there is a polynomial-time algorithm that computes the exact number of solutions of a #P-complete problem.
    - Such an algorithm would imply P $=$ NP.
- Therefore, it is interesting to find an approximation scheme, such as an FPRAS, for counting satisfying assignments of a DNF formula.

Outline

A naïve sampling algorithm

- $c(F)$: the number of satisfying assignments of a DNF formula F.
- We assume $c(F) > 0$ (it is easy to check whether $c(F) = 0$ first).

DNF counting algorithm I

- **Input:** DNF formula F with n variables.
- **Output:** Y, as an approximation of $c(F)$.

```
1. $X \leftarrow 0$.
2. For $k \leftarrow 1$ to $m$:
    1. Generate a random assignment for the $n$ variables, chosen uniformly at
       random from all $2^n$ assignments.
    2. If the random assignment satisfies $F$, set $X \leftarrow X + 1$.
3. Return $Y \leftarrow (X/m)\, 2^n$.
```

Analysis of the naïve algorithm

- Let
$$X_k = \begin{cases} 1, & \text{if the } k\text{-th assignment satisfies } F, \\ 0, & \text{otherwise.} \end{cases}$$
- Then $\Pr[X_k = 1] = c(F)/2^n$.
- Let $X = \sum_{k=1}^{m} X_k$, so
$$\mathbb{E}[X] = m \cdot \frac{c(F)}{2^n}.$$
- Hence
$$\mathbb{E}[Y] = \frac{\mathbb{E}[X] \cdot 2^n}{m} = c(F),$$
i.e., Y is an unbiased estimator of $c(F)$.

Limitations of the naïve algorithm

Using Theorem 1 with $\mu = c(F)/2^n$:

- We need
$$m \geq \frac{3 \cdot 2^n \ln(2/\Delta)}{\varepsilon^2 c(F)}.$$
- If $c(F) \geq 2^n/\alpha(n)$ for some polynomial α, then m is polynomial in n, $1/\varepsilon$ and $\ln(1/\Delta)$.
- But if $c(F) = \mathrm{poly}(n)$, then
$$m = \Theta\left(\frac{2^n}{c(F)}\right),$$
which is not necessarily polynomial.

Key issue

The set of satisfying assignments may be too sparse in the space of all 2^n assignments.

Revising the algorithm

- We revise the naïve algorithm to obtain an FPRAS.
- Let
$$F = C_1 \vee C_2 \vee \cdots \vee C_t$$
be a DNF formula, with clauses C_i.
- Assume w.l.o.g. that no clause contains both a variable and its negation.
- If clause C_i has ℓ_i literals, then there are exactly $2^{n-\ell_i}$ satisfying assignments for C_i.

Sets S_{C_i}, U and S

- Let S_{C_i} be the set of assignments that satisfy clause C_i.
- Define a set for "over-estimate":

$$U = \{(i, a) : 1 \leq i \leq t,\ a \in S_{C_i}\}.$$

- Then

$$|U| = \sum_{i=1}^{t} |S_{C_i}|.$$

- We want to estimate

$$c(F) = \left| \bigcup_{i=1}^{t} S_{C_i} \right| .$$

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Clearly $c(F) \le |U|$.

($\because$ an assignment satisfying multiple clauses appears multiple times in U.)

Defining a dense subset S

- Construct a subset $S \subseteq U$ that has exactly one pair for each satisfying assignment of F.
- For each satisfying assignment a of F, choose the smallest index i such that $a \in S_{C_i}$ and include (i, a) in S.
- Formally,

$$S = \{(i, a) : 1 \leq i \leq t,\ a \in S_{C_i},\ a \notin S_{C_j} \text{ for } j < i\}.$$

- Then $|S| = c(F)$.

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- Then $|S| = c(F)$.
- Moreover, each assignment can satisfy at most t clauses, so

$$\frac{|S|}{|U|} \ge \frac{1}{t},$$

i.e., S is relatively dense in U.

An Illustrating Example (1/4)

- Consider three variables x_1, x_2, x_3 and the DNF formula

$$F = C_1 \vee C_2 \vee C_3,$$

where

$$C_1 = x_1 \wedge x_2, \quad C_2 = x_2 \wedge x_3, \quad C_3 = x_1 \wedge x_3.$$

- An assignment $a = (x_1, x_2, x_3) \in \{0,1\}^3$ satisfies C_i iff:

$$S_{C_1} = \{110, 111\}, \quad S_{C_2} = \{011, 111\}, \quad S_{C_3} = \{101, 111\}.$$

- Satisfying assignments of F:

$$\bigcup_{i=1}^{3} S_{C_i} = \{110, 111, 011, 101\}.$$

- Hence the number of satisfying assignments is $c(F) = 4$.

An Illustrating Example (2/4): the over-estimate set U

- Recall the definition

$$U = \{(i,a) : 1 \le i \le t,\ \ a \in S_{C_i}\}.$$

- In our example, $t = 3$, so

$$U = \{(1,110),(1,111)\} \cup \{(2,011),(2,111)\} \cup \{(3,101),(3,111)\}.$$

- Thus $|U| = 6$.
- **Note:** the assignment 111 appears three times in U, once for each clause it satisfies.

An Illustrating Example (3/4): Constructing $S \subseteq U$

- For each satisfying assignment a of F, choose the *smallest* index i such that $a \in S_{C_i}$, and include (i, a) in S.
- For our four satisfying assignments:

a	clauses satisfied	chosen pair
110	C_1	$(1, 110)$
011	C_2	$(2, 011)$
101	C_3	$(3, 101)$
111	C_1, C_2, C_3	$(1, 111)$

- Hence

$$S = \{(1, 110),\ (2, 011),\ (3, 101),\ (1, 111)\}.$$

- Every satisfying assignment appears *exactly once* in S, so

$$|S| = 4 = c(F).$$

An Illustrating Example (4/4): Density of S inside U

- In general, each assignment can satisfy at most t clauses, so each assignment appears in at most t pairs in U.
- In our example, $t = 3$, and we found

$$|S| = 4, \qquad |U| = 6.$$

- Thus

$$\frac{|S|}{|U|} = \frac{4}{6} = \frac{2}{3} \geq \frac{1}{3} = \frac{1}{t}.$$

- This illustrates the general property:

$$\frac{|S|}{|U|} \geq \frac{1}{t},$$

i.e., S is relatively dense in U.

DNF counting algorithm II

DNF counting algorithm II (constructing S)

- **Input:** DNF formula F with n variables and clauses $C_1, \ldots, C_t$.
- **Output:** Y, an approximation of $c(F)$.

```
1. $X \leftarrow 0$.
2. For $k = 1$ to $m$:
    1. Choose $i \in \{1, 2, \ldots, t\}$ with probability $|S_{C_i}| / \sum_{j=1}^{t} |S_{C_j}|$, and then
       choose an assignment $a \in S_{C_i}$ uniformly at random.
    2. If $a$ does not satisfy any $C_j$ with $j < i$, then set $X \leftarrow X + 1$.
3. Return
       $$Y \leftarrow \frac{X}{m} \sum_{i=1}^{t} |S_{C_i}|.$$
```

Analysis of algorithm II

- For each pair (i, a) with $a \in S_{C_i}$:

$$\begin{aligned}\Pr[(i,a) \text{ is chosen}] &= \Pr[i \text{ is chosen}] \cdot \Pr[a \text{ is chosen} \mid i] \\ &= \frac{|S_{C_i}|}{|U|} \cdot \frac{1}{|S_{C_i}|} = \frac{1}{|U|}.\end{aligned}$$

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- So the indicator variables of "chosen pair is in S" have mean $\geq 1/t$.
- By Theorem 1, with

$$m = \left\lceil \frac{3t}{\varepsilon^2} \ln\left(\frac{2}{\Delta}\right) \right\rceil$$

we obtain an (ε, Δ)-approximation of $c(F)$.

Theorem 2

Theorem 2

- DNF counting algorithm II is an FPRAS for the DNF counting problem when
$$m = \left\lceil \frac{3t}{\varepsilon^2} \ln\left(\frac{2}{\Delta}\right) \right\rceil .$$
- The running time is polynomial in t, $1/\varepsilon$, and $\ln(1/\Delta)$.

Outline

Approximate uniform sampling

- We next present a *general reduction*:
  - If we can sample *almost uniformly* from the solution space of a self-reducible combinatorial problem, then we can approximately count the number of solutions.

Self-Reducible Combinatorial Problem

A problem where solutions for a large instance can be systematically reconstructed from solutions of polynomially many smaller instances of the same problem.

- We illustrate this technique for the problem of **counting independent sets in a graph.**

Independent Set

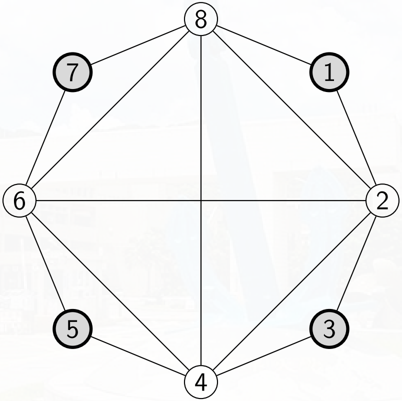

Fig.: $\{2, 4, 6, 8\}$ forms a clique and $\{1, 3, 5, 7\}$ is an independent set.

ϵ-uniform sample and FPAUS

Let Ω be a finite sample space and w be the (random) output of a sampling algorithm.

ε-uniform sample

The algorithm generates an ε-uniform sample of Ω if for any subset $S \subseteq \Omega$,

$$\Big| \Pr[w \in S] - |S|/|\Omega| \Big| \leq \varepsilon.$$

FPAUS

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

From FPAUS to FPRAS (independent sets)

- Consider an FPAUS for independent sets.
- Input: a graph $G = (V, E)$ and parameter ε.
- Sample space $\Omega(G)$: all independent sets in G.
- We want an FPRAS for $|\Omega(G)|$, the number of independent sets.

- Let $m = |E|$ and fix an ordering $e_1, e_2, \ldots, e_m$ of the edges.
- Let E_i be the set of the first i edges, $G_i = (V, E_i)$.
- Let $\Omega(G_i)$ be the set of independent sets in G_i.

⋆ **Note:** G_0 has no edges, so $|\Omega(G_0)| = 2^{|V|}$.

Decomposition of $|\Omega(G)|$

- Define ratios

$$r_i = \frac{|\Omega(G_i)|}{|\Omega(G_{i-1})|}, \qquad i = 1, 2, \ldots, m.$$

- Then

$$|\Omega(G)| = |\Omega(G_m)| = |\Omega(G_0)| \cdot \frac{|\Omega(G_1)|}{|\Omega(G_0)|} \cdot \frac{|\Omega(G_2)|}{|\Omega(G_1)|} \cdots \frac{|\Omega(G_m)|}{|\Omega(G_{m-1})|} = 2^n \prod_{i=1}^{m} r_i,$$

where $n = |V|$.

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where $n = |V|$.

- If we obtain good estimates $\hat{r}_i$ for each r_i, then

$$\widehat{|\Omega(G)|} = 2^n \prod_{i=1}^{m} \hat{r}_i$$

will be an approximation to $|\Omega(G)|$.

Lemma 1 (error control)

Lemma 1

Suppose that for all i, $1 \le i \le m$, the estimate $\hat{r}_i$ is an $(\varepsilon/(2m), \Delta/m)$-approximation for r_i. Let $R = \prod_{i=1}^{m} \frac{\hat{r}_i}{r_i}$. Then

$$\Pr\Big[|R-1| \le \varepsilon\Big] \ge 1 - \Delta.$$

Idea of proof:

- Apply the definition of (ε, Δ)-approximation to each $\hat{r}_i$.
- Use the union bound over all i.
- Bound the product $\prod_i (\hat{r}_i/r_i)$ using $(1 \pm x)$ estimates.

Proof of Lemma 1 (1/2)

- Let E_i be the event

$$E_i = \left\{ \left| \tilde{r}_i - r_i \right| \le \frac{\varepsilon}{2m} r_i \right\}.$$

Then by assumption $\Pr[E_i] \ge 1 - \Delta/m$ for each i.

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  Then by assumption $\Pr[E_i] \ge 1 - \Delta/m$ for each i.

- **Step 1: all estimates good with high probability.** Let $E = \bigcap_{i=1}^{m} E_i$. By the union bound,

$$\Pr[E] = 1 - \Pr[\neg E] \ge 1 - \sum_{i=1}^{m} \Pr[\neg E_i] \ge 1 - m \cdot \frac{\Delta}{m} = 1 - \Delta.$$

Proof of Lemma 1 (2/2)

- **Step 2: bound the product when all E_i hold.** On E_i we have

$$1 - \frac{\varepsilon}{2m} \le \frac{\tilde{r}_i}{r_i} \le 1 + \frac{\varepsilon}{2m}.$$

- Hence on E (assuming $0 < \varepsilon \le 1$),

$$\left(1 - \frac{\varepsilon}{2m}\right)^m \le R \le \left(1 + \frac{\varepsilon}{2m}\right)^m .$$

- Thus on E, $|R - 1| \le \varepsilon$. Since $\Pr[E] \ge 1 - \Delta$, we conclude

$$\Pr\left[|R - 1| \le \varepsilon\right] \ge 1 - \Delta.$$

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- Hence on E (assuming $0 < \varepsilon \le 1$),

$$1-\varepsilon \le (1-\varepsilon/2) \le \left(1 - \frac{\varepsilon}{2m}\right)^m \le R \le \left(1 + \frac{\varepsilon}{2m}\right)^m \le (1+\varepsilon/2) \le 1+\varepsilon.$$

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$$\Pr\Big[|R-1| \le \varepsilon\Big] \ge 1 - \Delta.$$

Estimating r_i

Algorithm to estimate r_i

- **Input:** graphs $G_{i-1} = (V, E_{i-1})$ and $G_i = (V, E_i)$.
- **Output:** estimate $\hat{r}_i$ of r_i.

```
1 $X \leftarrow 0$.
2 Repeat for $M = \left\lceil 1296\, m^2 \varepsilon^{-2} \ln\left(\frac{2m}{\Delta}\right) \right\rceil$ independent trials:
    a Generate an $(\varepsilon/(6m))$-uniform sample from $\Omega(G_{i-1})$.
    b If the sample is an independent set in $G_i$, set $X \leftarrow X + 1$.
3 Return $\hat{r}_i \leftarrow X/M$.
```

Lemma 2 (quality of $\hat{r}_i$)

Lemma 2

When $m \geq 1$ and $0 < \varepsilon \leq 1$, the above procedure for estimating r_i yields an $(\varepsilon/(2m), \Delta/m)$-approximation for r_i.

Sketch of proof:

- Show that $r_i = |\Omega(G_i)|/|\Omega(G_{i-1})| \geq 1/2$: adding a single edge removes at most half of the independent sets.
- Use the ε-uniformity of the sampler to bound the bias of $\hat{r}_i$:

$$\left|\mathbb{E}[\hat{r}_i] - r_i\right| \leq \frac{\varepsilon}{6m}.$$

- Apply Theorem 1 with appropriate parameters and combine bounds to obtain the $(\varepsilon/(2m), \Delta/m)$ guarantee.

Lemma 2 – Proof (1)

Step 1: $r_i \geq 1/2$.

- G_i is obtained from G_{i-1} by adding a single edge $e_i = (u, v)$.
- **Note:** An independent set in G_i is also an independent set in G_{i-1}.
- Each independent set in $\Omega(G_{i-1}) \setminus \Omega(G_i)$ contains both u and v.

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- **Note:** An independent set in G_i is also an independent set in G_{i-1}.
- Each independent set in $\Omega(G_{i-1}) \setminus \Omega(G_i)$ contains both u and v.
    - Independent sets disappear due to the newly added edge (u, v).

Lemma 2 – Proof (1) (contd.)

- Associate each $I \in \Omega(G_{i-1}) \setminus \Omega(G_i)$ with an independent set $I \setminus \{v\} \in \Omega(G_i)$.
- In this mapping, note that $I' \in \Omega(G_i)$ is associated with no more than one independent set $I' \cup \{v\} \in \Omega(G_{i-1}) \setminus \Omega(G_i)$, thus $|\Omega(G_{i-1}) \setminus \Omega(G_i)| \leq |\Omega(G_i)|$.

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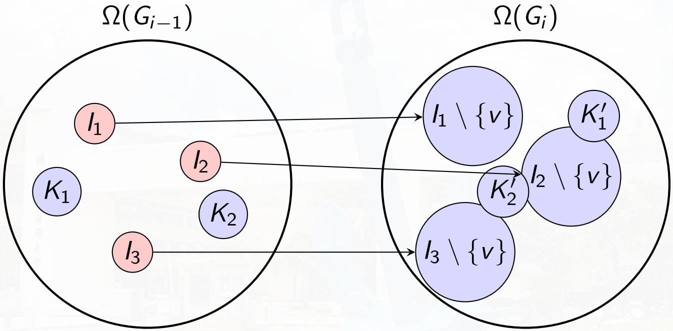
- It follows that

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

- Hence at most half of the independent sets of G_{i-1} are removed:

Lemma 2 – Injection idea



$I_1, I_2, I_3 \in \Omega(G_{i-1}) \setminus \Omega(G_i)$
(sets containing both u and v)

$\Omega(G_i)$ contains all images $I_j \setminus \{v\}$
and possibly more independent sets

Each removed set I is mapped injectively to $I \setminus \{v\} \in \Omega(G_i)$, so
$$|\Omega(G_{i-1}) \setminus \Omega(G_i)| \leq |\Omega(G_i)|.$$

Lemma 2 – Proof (2)

Step 2: bias from almost-uniform sampling.

- Let μ be the probability that one sample from the $(\varepsilon/(6m))$-uniform sampler for $\Omega(G_{i-1})$ lies in $\Omega(G_i)$.
- Since the sampler is $\varepsilon/(6m)$-uniform,

$$|\mu - r_i| \le \frac{\varepsilon}{6m}.$$

- From $r_i \ge 1/2$ we also get a relative bound

$$|\mu - r_i| \le \frac{\varepsilon}{6m} \cdot 2 \cdot \frac{1}{2} \le \frac{\varepsilon}{3m} r_i.$$

and $\mu \ge r_i - \dfrac{\varepsilon}{6m} \ge \dfrac{1}{2} - \dfrac{\varepsilon}{6m} \ge \dfrac{1}{3}$.

Lemma 2 – Proof (3)

Step 3: Chernoff bound for the sampling error.

- Let $Y_1, Y_2, \ldots, Y_M$ be independent indicators of the event "sample is in $\Omega(G_i)$"; then $X = \sum_{j=1}^{M} Y_j$, $\hat{r}_i = X/M$, and $\mathbb{E}[Y_j] = \mathbb{E}[\hat{r}_i] = \mu$.

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- By the Chernoff bound, for $0 < \delta \leq 1$,

$$\Pr\Big[\big|\hat{r}_i - \mu\big| \geq \delta\mu\Big] \leq 2\exp\left(-\frac{\delta^2 \mu M}{3}\right).$$

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- Use $\delta = \varepsilon/(8m)$ and our finding that $\mu \ge 1/3$, we have

$$\Pr\left[\left|\hat{r}_i - \mu\right| \ge \frac{\varepsilon}{8m}\,\mu\right] \le 2\exp\left(-\frac{\varepsilon^2 M}{576\, m^2}\right).$$

Lemma 2 – Proof (3) (contd.)

$$\Pr\left[\left|\hat{r}_i - \mu\right| \geq \frac{\varepsilon}{8m}\,\mu\right] \leq 2\exp\left(-\frac{\varepsilon^2 M}{576\, m^2}\right).$$

- Our choice:

$$M = \left\lceil 1296\, m^2 \varepsilon^{-2} \ln\left(\frac{2m}{\Delta}\right)\right\rceil \;\geq\; 576\, m^2 \varepsilon^{-2} \ln\left(\frac{2m}{\Delta}\right)$$

  guarantees

$$\Pr\left[\left|\hat{r}_i - \mu\right| \geq \frac{\varepsilon}{8m}\,\mu\right] \leq \frac{\Delta}{m}.$$

Lemma 2 – Proof (4)

Step 4: combine the two errors.

- On the "good" event from Step 3, $\left|\hat{r}_i - \mu\right| \leq \frac{\varepsilon}{8m}\,\mu.$ (w.h.p.).
- Together with Step 2, $|\mu - r_i| \leq \frac{\varepsilon}{6m}$, and using $r_i \geq 1/2$ and μ close to r_i, a straightforward calculation shows

$$\left|\hat{r}_i - r_i\right| \leq \frac{\varepsilon}{2m}\, r_i.$$

- Therefore

$$\Pr\left[\left|\hat{r}_i - r_i\right| \leq \frac{\varepsilon}{2m}\, r_i\right] \geq 1 - \frac{\Delta}{m}.$$

Outline

FPAUS $\rightarrow$ FPRAS

Theorem 3

Given an FPAUS for independent sets in any graph, we can construct an FPRAS for the number of independent sets in a graph G.

- Reason:
    - Use the FPAUS to approximately estimate each r_i.
    - Apply Lemma 2 for each r_i and Lemma 1 to control the product.
    - The number of samples M is polynomial in m, $1/\varepsilon$, and $\ln(1/\Delta)$, and each sample takes polynomial time.

How to get an FPAUS?

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How to get an FPAUS?

- We have reduced approximate counting to (almost) uniform sampling.
- For independent sets, how do we obtain an FPAUS?
- One approach:
  - Use Markov Chain Monte Carlo (MCMC) with a carefully designed chain.
  - See coupling of Markov chains, e.g. Ch. 12 of [MU17].

Markov Chain Monte Carlo (MCMC)

- MCMC provides a general approach to sampling from a desired distribution.
- Basic idea:
  - Define an ergodic Markov chain whose state space is the **sample space**.
  - Ensure that its stationary distribution equals the desired distribution.
- Let $X_0, X_1, \ldots, X_n$ be a run of the chain.
- For a sufficiently large number of steps $\boldsymbol{r}$, the distribution of X_r is close to the stationary distribution and can be used as a **sample**.

MCMC sampling

- Repeating the argument, we can use $X_r, X_{2r}, X_{3r}, \dots$ as (almost) independent samples from the stationary distribution.
- Efficiency of MCMC depends on:
  - How large r must be (**mixing time**).
  - Cost per step of the Markov chain.
- We focus on constructing efficient Markov chains with:
  - The desired stationary distribution (often uniform).
  - Small mixing time (for a rigorous FPAUS, we need mixing-time bounds).

Independent sets as states

- Let $G = (V, E)$ be a graph.
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    - Two states (independent sets) x and y are neighbors if they differ in exactly one vertex.
- This neighbor relation makes the state space **irreducible**.

Independent sets as states

- Let $G = (V, E)$ be a graph.
- State space: all independent sets of G.
- Neighbor relation:
  - Two states (independent sets) x and y are neighbors if they differ in exactly one vertex.
- This neighbor relation makes the state space **irreducible**.
  - Any independent set can be reached from the empty set by a sequence of vertex additions.
  - Conversely, we can delete vertices to reach the empty set.

Establish of the transition probabilities

- Next we need to establish the **transition probabilities**.
- A naïve approach: simple random walk on the state graph.

Establish of the transition probabilities

- Next we need to establish the **transition probabilities**.
- A naïve approach: simple random walk on the state graph.
- But this typically yields a stationary distribution where the probability of a state is proportional to its degree in the state graph.
- We need to modify the transition probabilities to get a uniform stationary distribution.

Towards a uniform stationary distribution

Lemma 3

- For a finite state space Ω with neighbor sets $N(x)$, if we choose transitions as

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

for some $M \geq \max_{x \in \Omega} |N(x)|$, then, assuming irreducibility and aperiodicity, the stationary distribution is uniform.

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  for some $M \geq \max_{x \in \Omega} |N(x)|$, then, assuming irreducibility and aperiodicity, the stationary distribution is uniform.

- That is, if we modify the random walk by giving each vertex an appropriate self-loop probability, then we can obtain a uniform stationary distribution.

Proof of Lemma 3

- For any $x \neq y$, since $\pi_x = \pi_y$ and $P_{x,y} = P_{y,x}$ $(=1/M)$, we have

$$\pi_x P_{x,y} = \pi_y P_{y,x}.$$

- Then, by applying the following theorem, it follows that the uniform distribution is the stationary distribution.

Theorem 4 (recall)

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

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

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

Example chain for independent sets

- Consider the following simple Markov chain:

1. X_0 is an arbitrary independent set in G.
2. To get X_{i+1} from X_i:
    1. Choose a vertex $v \in V$ uniformly at random.
    2. If $v \in X_i$, set $X_{i+1} = X_i \setminus \{v\}$.
    3. If $v \notin X_i$ and $X_i \cup \{v\}$ is independent, set $X_{i+1} = X_i \cup \{v\}$.
    4. Otherwise, set $X_{i+1} = X_i$.

- The chain is irreducible and aperiodic.
- The stationary distribution can be shown to be uniform over independent sets, by applying Lemma 3.

Non-uniform stationary distributions

- Sometimes we want to sample according to a non-uniform distribution.
- Example: distributions where probability is proportional to some weight function.

Non-uniform stationary distributions

- Sometimes we want to sample according to a non-uniform distribution.
- Example: distributions where probability is proportional to some weight function.
- **Solution:** Use the **Metropolis algorithm.**

The Metropolis algorithm

- Given a connected state space Ω with neighbor structure $\{N(x) \mid x \in \Omega\}$.
- Desired stationary distribution:

$$\pi_x = \frac{b(x)}{B}, \quad B = \sum_{y \in \Omega} b(y), \quad b(x) > 0.$$

- The Metropolis chain:

$$P_{x,y} = \begin{cases} \frac{1}{M} \min\left(1, \frac{\pi_y}{\pi_x}\right), & x \neq y,\ y \in N(x), \\ 0, & x \neq y,\ y \notin N(x), \\ 1 - \sum_{z \neq x} P_{x,z}, & x = y, \end{cases}$$

for some $M \geq \max_{x \in \Omega} |N(x)|$.

- Under irreducibility and aperiodicity, the stationary distribution is π.

Correctness of the Metropolis algorithm

- For $x \neq y$ with $y \in N(x)$,

$$P_{x,y} = \frac{1}{M}\min\left(1, \frac{\pi_y}{\pi_x}\right), \quad P_{y,x} = \frac{1}{M}\min\left(1, \frac{\pi_x}{\pi_y}\right).$$

- For any $x \neq y$, suppose first that $\pi_x \leq \pi_y$. Then

$$P_{x,y} = \frac{1}{M}, \quad P_{y,x} = \frac{1}{M}\frac{\pi_x}{\pi_y}.$$

Hence

$$P_{x,y} = \frac{1}{M} = \frac{\pi_y}{\pi_x}P_{y,x} \implies \pi_x P_{x,y} = \pi_y P_{y,x}.$$

- The case $\pi_x > \pi_y$ can be similarly proved.
- For $x = y$ the equality $\pi_x P_{x,x} = \pi_x P_{x,x}$ is trivial.
- Thus, for all states x, y, $\pi_x P_{x,y} = \pi_y P_{y,x}$.

Example: independent sets with **weights**

- Let states be independent sets I in G.
- For a parameter $\lambda > 0$, define

$$\pi_x \propto \lambda^{|I_x|},$$

where I_x is the independent set of state x.
- That is,

$$\pi_x = \frac{\lambda^{|I_x|}}{\sum_y \lambda^{|I_y|}}.$$

- When $\lambda = 1$, this reduces to the uniform distribution.

Metropolis chain for weighted independent sets

1. X_0 is an arbitrary independent set.
2. To compute X_{i+1} from X_i:
    1. Choose a vertex $v \in V$ uniformly at random (so $M = |V|$).
    2. If $v \in X_i$, propose $Y = X_i \setminus \{v\}$ and accept with probability $\min(1, 1/\lambda)$.
    3. If $v \notin X_i$ and $X_i \cup \{v\}$ is independent, propose $Y = X_i \cup \{v\}$ and accept with probability $\min(1, \lambda)$.
    4. Otherwise, stay at X_i.

- For this chain, the stationary distribution is the desired $\pi_x \propto \lambda^{|I_x|}$.
- Note: we only ever need the ratios π_y/π_x, not the normalizing constant B.

Remarks

- For both uniform and weighted cases, we design a Markov chain whose stationary distribution is the one we want.
- Using coupling and mixing-time analysis (e.g., via ch. 12 in [MU17]), we can obtain an FPAUS.
- Combined with the reduction via ratios r_i, this yields FPRASs for certain counting problems.

Discussions