Monte Carlo Methods

collection of tools for estimating values thru sampling & estimation

(ε, δ) Approximation

A randomized alg gives an (ε,δ) approx for value V
if the output X of the alg satisfies
$$\Pr(|X-V| > \varepsilon|V|) \leq \delta$$

Monte Carlo Thm

Let $X_1, X_2, \dots, X_m$ iid. Bernoulli with $E(X_i)=\mu$

If $m \geq \frac{3\ln(\frac{2}{\delta})}{\varepsilon^2 \mu}$ then

$$\Pr\left(\left|\frac{1}{m}\sum_{i=1}^{m} X_i - \mu\right| \geq \varepsilon\mu\right) \leq \delta$$

Pf: Chernoff bounds

#P complexity class associated with counting solns to problems in NP

#P complete problems:

- # indep sets in a graph
- # satisfying assignments to DNF formula
- # perfect matchings in a bipartite graph

Fully polynomial randomized approx scheme FPRAS

a randomized alg for which, given an input x and any parameters ε & δ with $0<\varepsilon,\delta<1$, the alg outputs an (ε,δ) approx to $V(x)$ in time poly in $\frac{1}{\varepsilon}$, $\ln\frac{1}{\delta}$ & size of input

Note: suffices to take $\delta = \frac{1}{4}$
because easy to boost error prob:
Run $k = 16\log\left(\frac{2}{\delta}\right)$ trials w. error prob $\frac{1}{4}$ $\Longrightarrow$ $y_1, y_2, \dots, y_k$

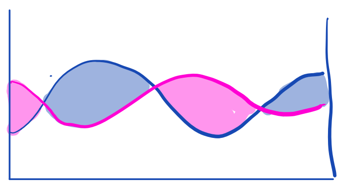
Let $m = \text{median}(y_1, \dots, y_k)$

Then $\Pr\left[m \notin (1 \pm \varepsilon) V(x)\right] \le \delta$ by Chernoff

Want to sample from some set (e.g. ISs of graph G)
where π is desired distribution $\pi_I = \Pr(\text{output IS } I)$
(often π uniform distn)

Definition
total variation distance between 2 distns on some sample space Ω

$$\|D_1 - D_2\|_{TV} = \frac{1}{2}\sum_{x \in \Omega} |D_1(x) - D_2(x)| = \max_{A \subseteq \Omega} |D_1(A) - D_2(A)|$$



$\|D_1 - D_2\|_{TV}$ = pink area = blue area

For sampling problems, we seek

$\boxed{\text{FPAUS - fully polynomial almost uniform sampler}}$

Input: x, ε $\longrightarrow$ FPAUS (Fully polynomial almost uniform sampler) $\longrightarrow$ outputs samples from $\Omega(x)$ sampled from distn μ
s.t. $d_{TV}(\mu, \pi) \le \varepsilon$

runs in time polynomial in size of x & $\ln\left(\frac{1}{\varepsilon}\right)$

Approximate counting $\Longleftrightarrow$ Approximate Sampling
FPRAS FPAUS

self reducible problems
randomized reduction from
problems of size k
to problems of size $k-1$

Lemma Given FPAUS for sampling indep sets of graph G, we can construct FPRAS for estimating $|\Omega(G)|$
ISs.

Pf Want estimate $\bar{\Omega}$ of $|\Omega(G)|$

$$\Pr\left(|\bar{\Omega} - |\Omega(G)|| \geq \varepsilon |\Omega(G)| \right) \leq \delta$$

$G=(V,E)$ $e_1, e_2, \ldots, e_m$ arbitrary ordering of edges

$E_i = \{e_1, e_2, \ldots, e_i\}$ $G_i = (V, E_i)$ $G_m = G$ $G_0 = (V, \phi)$

$\Omega(G_i)$: set of ISs in G_i

$$|\Omega(G)| = \frac{|\Omega(G_m)|}{|\Omega(G_{m-1})|} \times \frac{|\Omega(G_{m-1})|}{|\Omega(G_{m-2})|} \times \cdots \times \frac{|\Omega(G_1)|}{|\Omega(G_0)|} \times \underbrace{|\Omega(G_0)|}_{2^n}$$

Let $r_i = \dfrac{|\Omega(G_i)|}{|\Omega(G_{i-1})|}$

$$|\Omega(G)| = \prod_{i=1}^{m} r_i \, 2^n$$

Observation: $\frac{1}{2} \leq r_i \leq 1$

G_i has one extra edge, say (u,v)

$$\Omega(G_i) \subseteq \Omega(G_{i-1})$$

Can't sample from uniform distn on $\Omega(G_{i-1})$
but can use FPAUS

Two errors we need to bound:

(1) FPAUS $\neq$ exact sampler so exp value $\neq r_i$

But using, say, $\frac{\varepsilon}{6m}$ sampler $\quad |E(\tilde{r}_i) - r_i| \leq \frac{\varepsilon}{6m}$

(2) With samples we get approx to $E(\tilde{r}_i)$

since r_i big $(\geq \frac{1}{2})$, $E(\tilde{r}_i)$ big $\Rightarrow$

Monte Carlo Thm $\Rightarrow$ $O\left(\frac{m^2}{\varepsilon^2} \ln\left(\frac{1}{\delta}\right)\right)$ samples suffice

From these bound $R = \prod_{i=1}^{m} \frac{\tilde{r}_i}{r_i}$

$\boxed{\text{Claim:}}$ If $\tilde{r}_i$ is $\left(\frac{\varepsilon}{2m}, \frac{\delta}{m}\right)$ approx to r_i $\forall i$

then X is (ε, δ) approx to $|\Omega(G)|$

$\Uparrow$

$\prod_{i=1}^{m} \tilde{r}_i \, 2^n$

Pf: $\quad \Pr\left(|\tilde{r}_i - r_i| \leq \frac{\varepsilon}{2m} r_i\right) \geq 1 - \frac{\delta}{m} \quad \forall i$

$\Rightarrow r_i\left(1 - \frac{\varepsilon}{2m}\right) \leq \tilde{r}_i \leq r_i\left(1 + \frac{\varepsilon}{2m}\right) \quad$ w.p. $\geq 1 - \frac{\delta}{m}$

$\Rightarrow \left(1 - \frac{\varepsilon}{2m}\right) \leq \frac{\tilde{r}_i}{r_i} \leq \left(1 + \frac{\varepsilon}{2m}\right)$

$1 - \varepsilon \leq \left(1 - \frac{\varepsilon}{2m}\right)^m \leq \prod_{i=1}^{m} \frac{\tilde{r}_i}{r_i} \leq \left(1 + \frac{\varepsilon}{2m}\right)^m \leq 1 + \varepsilon \quad$ w.p. $\geq 1 - \delta$

$(1-\varepsilon) \prod_{i=1}^{m} r_i \leq \prod_{i=1}^{n} \tilde{r}_i \leq (1+\varepsilon) \prod_{i=1}^{m} r_i \quad$ w.p. $1 - \delta$

$\equiv \Pr\left(\left|\prod_{i=1}^{m} \tilde{r}_i - \prod_{i=1}^{m} r_i\right| \geq \varepsilon \prod_{i=1}^{m} r_i\right) \leq \delta$

How to sample elts from a universe Ω with $|U|=n$ according to distn $\pi=(\pi_1,\dots,\pi_n)$?

Cool idea: design MC whose state space is Ω that has stationary distn π

- simulate MC until it "mixes"
- use state at that time as sample

2 key questions:

(1) how to design chain w/ right π?

(2) how to bound mixing time?

Example: sampling indep sets uniformly from $G=(V,E)$

states: indep sets

X_t: some indep set

MC:

choose vertex v u.a.r. from V

if $v \in X_t$, then $X_{t+1} := X_t \setminus v$

if $v \notin X_t$ and can be added without violating independence then $X_{t+1} := X_t \cup v$

otherwise $X_{t+1} := X_t$

Claim:

- MC irreducible
- if $\exists$ edge then aperiodic
- stationary distn uniform (chain doubly stochastic)

$P_{I,I'} = P_{I',I}$ $[\frac{1}{n}$ or $0]$

General technique: given Ω and a connected graph on Ω define transition prob s so that will have stationary distn π

$\boxed{\text{Metropolis Algorithm}}$

Input: Ω; connected graph $G=(\Omega,E)$, π s.t. $\sum_{i\in\Omega}\pi_i=1$, $\pi_i>0$

Bounding mixing time

① Spectral gap, conductance, expansion

② coupling

⋮

Coupling

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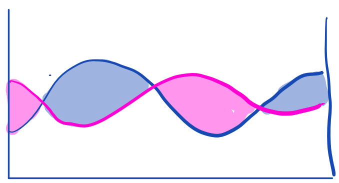

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Ω

Common defn of mixing time $\tau(\varepsilon)$

$$\tau(\varepsilon) = \min \{ t \mid \|P^t - \pi\|_{TV} \le \varepsilon \}$$

say MC is rapidly mixing if $\tau(\varepsilon)$ polynomial in $\log|\Omega|$ and $\log(\frac{1}{\varepsilon})$

(we know this is related to spectral gap)

$\boxed{\text{Coupling}}$ simple & elegant approach to bounding mixing time

Given a MC on Ω, a coupling is a MC on $\Omega \times \Omega$ defining stochastic process (X_t, Y_t) s.t.

① each of X_t & Y_t in isolation is faithful copy of MC

② If $X_t = Y_t$ then $X_{t+1} = Y_{t+1}$

$\boxed{\text{Coupling Lemma}}$ Let (X_t, Y_t) be a coupling

Suppose $\exists\, T$ s.t. $\forall x, y$

$$\Pr(X_T \neq Y_T \mid X_0 = x, Y_0 = y) \leq \varepsilon$$

Then $\tau(\varepsilon) \leq T$

Examples:

(1) Random walk on hypercube $N = 2^n$ nodes

in each step, choose random coordinate i, random bit $b \in \{0,1\}$

change i^{th} bit to b

② Indep sets of fixed size k here distances may $\uparrow$

Chain: choose vertex $v \in X_t$ u.a.r. & a vertex $w \in V$ u.a.r.

If $w \notin X_t$ & $X_t - v + w$ indep then $X_{t+1} = X_t - v + w$

else $X_{t+1} = X_t$

<u>Claim:</u> MC rapidly mixing if $k \le \frac{n}{3\Delta+3}$