Sampling & Counting for Big Data

南京大学 尹一通

2019年全国理论计算机科学学术年会 2019年8月3日于兰州大学

Sampling vs Counting

[Jerrum-Valiant-Vazirani '86]: for all self-reducible problems





RANDOM GENERATION OF COMBINATORIAL STRUCTURES FROM A UNIFORM DISTRIBUTION

Mark R. JERRUM Department of Computer Science, University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom

Leslie G. VALIANT * Aiken Computation Laboratory, Harvard University, Cambridge, MA 02138, U.S.A.

Vijay V. VAZIRANI ** Computer Science Department, Cornell University, Ithaca, NY 14853, U.S.A.

MCMC Sampling

Markov chain for sampling $X = (X_1, X_2, ..., X_n) \sim \mu$

• Gibbs sampling (Glauber dynamics, heat-bath)

pick a random *i*; resample $X_i \sim \mu_v(\cdot | N(v))$; [Glauber, '63] [Geman, Geman, '84]

Metropolis-Hastings algorithm

pick a random *i*; propose a random *c*; $X_i = c$ w.p. $\propto \mu(X')/\mu(X)$;

[Metropolis *et al*, '53] [Hastings, '84]

• Analysis: coupling methods

[Aldous, '83] [Jerrum, '95] [Bubley, Dyer '97] may give O(*n* log *n*) upper bound for *mixing time*

Computational Phase Transition

hardcore model: graph G(V,E), max-degree Δ , fugacity $\lambda > 0$

approx sample independent set I in G w.p. $\propto \lambda^{|I|}$



- [Weitz, **STOC**'06]: If $\lambda < \lambda_c$, $n^{O(\log \Delta)}$ time.
- [Sly, FOCS'10 best paper]: If $\lambda > \lambda_c$, NP-hard even for $\Delta = O(1)$.

[Efthymiou, Hayes, Štefankovič, Vigoda, Y., FOCS'16]: If $\lambda < \lambda_c$, O(*n* log *n*) mixing time. If Δ is large enough, and there is no small cycle.

A phase transition occurs at λ_c .



Big Data?

Sampling and Inference for Big Data

- Sampling from a joint distribution (specified by a probabilistic graphical model).
- Inferring according to a probabilistic graphical model.
- The data (probabilistic graphical model) is BIG.



Parallel/distributed algorithms for sampling?

- PTIME ⇒ Polylog(n) rounds
- For parallel/distributed computing:
 sampling = approx counting/inference?
 - PTIME => Polylog(n) rounds
- Dynamic sampling algorithms?
 - PTIME => Polylog(n) incremental cost

Local Computation

"What can be computed locally?" [Noar, Stockmeyer, STOC'93, SICOMP'95]

the **LOCAL** model [Linial '87]:

- Communications are synchronized.
- In each round: unlimited local computation and communication with neighbors.
- Complexity: # of rounds to terminate in the worst case.



• In t rounds: each node can collect information up to distance t.

PLOCAL: t = polylog(n)

"What can be sampled locally?"

- Joint distribution defined by local constraints:
 - Markov random field
 - Graphical model
- Sample a random solution from the joint distribution:
 - distributed algorithms
 (in the *LOCAL* model)



network G(V,E)

Q: "What locally definable joint distributions are locally sample-able?"

MCMC Sampling

Classic MCMC sampling:

Markov chain $X_t \rightarrow X_{t+1}$:

pick a uniform random vertex v;

update X(v) conditioning on X(N(v));

 $O(n \log n)$ time when mixing

Parallelization:



- Chromatic scheduler [folklore] [Gonzalez *et al.*, AISTAT'11]: Vertices in the same color class are updated in parallel.
 - $O(\Delta \log n)$ mixing time (Δ is max degree)
- "Hogwild!" [Niu, Recht, Ré, Wright, NIPS'11][De Sa, Olukotun, Ré, ICML'16]: All vertices are updated in parallel, ignoring concurrency issues.
 - Wrong distribution!

Crossing the Chromatic # Barrier



Do not update adjacent vertices simultaneously. It takes $\geq \chi$ steps to update all vertices at least once.

Q: "How to update all variables simultaneously and still converge to the correct distribution?"

Markov Random Fields (MRF)

$$\forall \sigma \in [q]^V : \quad \mu(\sigma) \propto \prod_{v \in V} \nu_v(\sigma_v) \prod_{e=(u,v) \in E} \phi_e(\sigma_u, \sigma_v)$$

- Each vertex v∈V: a variable over domain [q] with distribution U_v
- Each edge e=(u,v)∈E: a symmetric binary constraint:

 $\phi_e:[q]\times[q]\to[0,1]$



The Local-Metropolis Algorithm

[Feng, Sun, Y., What can be sample locally? PODC'17]



Markov chain $X_t \rightarrow X_{t+1}$:

each vertex $v \in V$ independently proposes a random $\sigma_v \sim \nu_v$; each edge e=(u,v) passes its check independently with prob: $\phi_e(X_u, \sigma_v) \cdot \phi_e(\sigma_u, X_v) \cdot \phi_e(\sigma_u, \sigma_v)$; each vertex $v \in V$ update X_v to σ_v if all its edges pass checks;

• Local-Metropolis converges to the correct distribution μ .

The Local-Metropolis Algorithm

[Feng, Sun, Y., What can be sample locally? PODC'17]

each vertex $v \in V$ independently proposes a random $\sigma_v \sim \nu_v$; each edge e=(u,v) passes its check independently with prob: $\phi_e(X_u, \sigma_v) \cdot \phi_e(\sigma_u, X_v) \cdot \phi_e(\sigma_u, \sigma_v)$; each vertex $v \in V$ update X_v to σ_v if all its edges pass checks;

• Local-Metropolis converges to the correct distribution μ .

MRF:
$$\mu(\sigma) \propto \prod_{v \in V} \nu_v(\sigma_v) \prod_{e=(u,v) \in E} \phi_e(\sigma_u, \sigma_v)$$

- under coupling condition for *Metropolis-Hastings*:
 - Metropolis-Hastings: O(n log n) time
 - (lazy) Local-Metropolis: O(log n) time

Lower Bounds

[Feng, Sun, Y., What can be sample locally? PODC'17]

Approx sampling from any MRF requires $\Omega(\log n)$ rounds.

• for sampling: $O(\log n)$ is the new criteria of "local"

If $\lambda > \lambda_c$, sampling from hardcore model requires $\Omega(diam)$ rounds.



strong separation: sampling vs other local computation tasks

- Independent set is trivial to construct locally (e.g. \emptyset).
- The lower bound holds not because of the locality of information, but because of the locality of correlation.

Parallel/distributed algorithms for sampling?

- PTIME => Polylog(n) rounds
- For parallel/distributed computing:
 sampling = approx counting/inference?
 - PTIME ⇒ Polylog(n) rounds

Openation of the state of th

PTIME => Polylog(n) incremental cost

Example: Sample Independent Set (hardcore model)

 μ : distribution of independent sets I in $G \propto \lambda^{|I|}$

- Y∈ {0,1}^V indicates an independent set
- Each $v \in V$ returns a $Y_v \in \{0,1\}$, such that $Y = (Y_v)_{v \in V} \sim \mu$
- **Or**: $d_{\text{TV}}(Y, \mu) < 1/\text{poly}(n)$



Inference (Local Counting)

 μ : distribution of independent sets I in $G \propto \lambda^{|I|}$

 μ_v^{σ} : marginal distribution at v conditioning on $\sigma \in \{0,1\}^{S}$.

$$\forall y \in \{0, 1\}: \quad \mu_v^{\sigma}(y) = \Pr_{\mathbf{Y} \sim \mu}[Y_v = y \mid Y_S = \sigma]$$

- Each $v \in S$ receives σ_v as input.
- Each $v \in V$ returns a marginal distribution $\hat{\mu}_v^{\sigma}$ such that:

$$d_{\mathrm{TV}}(\hat{\mu}_v^{\sigma}, \mu_v^{\sigma}) \le \frac{1}{\mathrm{poly}(n)}$$

$$\frac{1}{Z} = \mu(\emptyset) = \prod_{i=1}^{n} \Pr_{\mathbf{Y} \sim \mu} [Y_{v_i} = 0 \mid \forall j < i : Y_{v_j} = 0]$$

Z: partition function (counting)



Decay of Correlation

 μ_v^{σ} : marginal distribution at v conditioning on $\sigma \in \{0,1\}^{S}$.

strong spatial mixing (SSM):

 \forall boundary condition $B \in \{0,1\}^{r-\text{sphere}(v)}$:

 $d_{\mathrm{TV}}(\mu_v^{\sigma}, \mu_v^{\sigma, B}) \le \mathrm{poly}(n) \cdot \exp(-\Omega(\mathbf{r}))$



SSM (iff $\lambda \leq \lambda_c$ when μ is the hardcore model) approx. inference is solvable in O(log *n*) rounds in the *LOCAL* model

Locality of Counting & Sampling [Feng, Y., PODC'18]

For all self-reducible graphical models:



Locality of Sampling



sequential O(log *n*)-local procedure:

- scan vertices in V in an arbitrary order $v_1, v_2, ..., v_n$
- for i=1,2,...,n: sample Y_{v_i} according to $\hat{\mu}_{v_i}^{Y_{v_1},...,Y_{v_{i-1}}}$

Network Decomposition

(C,D) -network-decomposition of G:

- classifies vertices into clusters;
- assign each cluster a color in [C];
- each cluster has diameter $\leq D$;
- clusters are properly colored.

 $(C,D)^r$ -ND: (C,D)-ND of G^r

Given a $(C,D)^r$ - ND:

sequential *r*-local procedure: $r = O(\log n)$

• scan vertices in V in an arbitrary order $v_1, v_2, ..., v_n$

• for $i=1,2,\ldots,n$: sample Y_{v_i} according to $\hat{\mu}_{v_i}^{Y_{v_1},\ldots,Y_{v_{i-1}}}$

can be simulated in O(CDr) rounds in LOCAL model



Network Decomposition

(C,D) -network-decomposition of G:

- classifies vertices into clusters;
- assign each cluster a color in [C];
- each cluster has diameter $\leq D$;
- clusters are properly colored.

 $(C,D)^r$ -ND: (C,D)-ND of G^r

 $(O(\log n), O(\log n))^r$ -ND can be constructed in $O(r \log^2 n)$ rounds w.h.p.



[Ghaffari, Kuhn, Maus, STOC'17]:

r-local SLOCAL algorithm:
 ∀ ordering π=(v₁, v₂, ..., v_n),
 returns random vector Y^(π)



 $O(r \log^2 n)$ -round LOCAL alg.: returns w.h.p. the $Y^{(\pi)}$ for some ordering π

Locality of Counting & Sampling [Feng, Y., PODC'18]

For all self-reducible graphical models:



Boosting Local Inference



• for $i=1,2,\ldots,n$: sample Y_{v_i} according to $\hat{\mu}_{v_i}^{Y_{v_1},\ldots,Y_{v_{i-1}}}$

multiplicative error: $\forall \sigma \in \{0,1\}^V$: $e^{-1/n^2} \le \frac{\hat{\mu}(\sigma)}{\mu(\sigma)} \le e^{1/n^2}$

SLOCAL JVV

Scan vertices in V in an arbitrary order v_1, v_2, \ldots, v_n : **pass 1:** sample $Y \in \{0,1\}^V$ by boosted sequential r-local sampler $\hat{\mu}$; $\forall \sigma \in [q]^V : e^{-1/n^2} \le \frac{\hat{\mu}(\sigma)}{\mu(\sigma)} \le e^{1/n^2}$ $r = O(\log n)$ **pass** 1': construct a sequence of ind. sets $\emptyset = Y_0, Y_1, \dots, Y_n = Y$; s.t. $\forall 0 \leq i \leq n$: • Y_i agrees with Y over v_1, \ldots, v_i • Y_i and Y_{i-1} differ only at v_i v_i samples $F_{v_i} \in \{0, 1\}$ independently with $\Pr[F_{v_i} = 0] = q_{v_i}$ where $q_{v_i} = \frac{\mu(\mathbf{Y}_{i-1})}{\hat{\mu}(\mathbf{Y}_i)} \cdot e^{-3/n^2} \in [e^{-5/n^2}, 1]$ Each $v \in V$ returns: $O(\log n)$ -local to compute • $Y_v \in \{0,1\}$ to indicate the ind. set;

• $F_v \in \{0,1\}$ indicate failure at v.

Scan vertices in V in an arbitrary order v_1, v_2, \ldots, v_n : **pass** 1: sample $Y \in \{0,1\}^V$ by boosted sequential *r*-local sampler $\hat{\mu}$; $\forall \sigma \in [q]^V : e^{-1/n^2} \le \frac{\hat{\mu}(\sigma)}{\mu(\sigma)} \le e^{1/n^2}$ $r = O(\log n)$ **pass** 1': construct a sequence of ind. sets $\emptyset = Y_0, Y_1, \ldots, Y_n = Y$; s.t. $\forall 0 \leq i \leq n$: • Y_i agrees with Y over v_1, \ldots, v_i • Y_i and Y_{i-1} differ only at v_i v_i samples $F_{v_i} \in \{0, 1\}$ independently with $\Pr[F_{v_i} = 0] = q_{v_i}$ where $q_{v_i} = \frac{\mu(\mathbf{Y}_{i-1})}{\hat{\mu}(\mathbf{Y}_i)} \cdot e^{-3/n^2} \in [e^{-5/n^2}, 1]$ $\forall \sigma \in \{0,1\}^V$: $\Pr[\mathbf{Y} = \sigma \land \forall i : F_{v_i} = 0] = \hat{\mu}(\sigma) \prod_{i=1}^{n} q_{v_i} = \hat{\mu}(\sigma) \prod_{i=1}^{n} \left(\frac{\hat{\mu}(\mathbf{Y}_{i-1})}{\hat{\mu}(\mathbf{Y}_i)} \cdot e^{-3/n^2} \right) \bigg|_{\mathbf{Y}}$

 $= \hat{\mu}(\sigma) \cdot \frac{\hat{\mu}(\emptyset)}{\hat{\mu}(\sigma)} \cdot e^{-\frac{3}{n}} \qquad \propto \begin{cases} \lambda^{\|\sigma\|_1} & \sigma \text{ is ind. set} \\ 0 & \text{otherwise} \end{cases}$

Locality of Counting & Sampling [Feng, Y., PODC'18]

For all self-reducible graphical models:



Local Exact Sampler

hardcore model: distribution of independent sets $I \propto \lambda^{|I|}$



[Feng, Sun, Y., **PODC**'17]:

If $\lambda > \lambda_c$, any approx sampler requires $\Omega(diam)$ rounds.



Hold for Big Data (local computation)!

Distributed Las Vegas Sampler

dynamic

sampler

Las Vegas (certifiable failure):

- Each $v \in V$ returns in **fixed** rounds:
 - local output $Y_v \in \{0,1\};$
 - local failure $F_v \in \{0,1\}$.
- Succeeds w.h.p.: $\sum_{v \in V} \mathbf{E}[F_v] = \mathbf{o}(1)$.
- Conditioning on success, $Y \sim \mu$.

Las Vegas (zero failure):

- Each $v \in V$ returns in random rounds:
 - local output $Y_v \in \{0,1\}$.
- Correctness: $Y \sim \mu$.



Parallel/distributed algorithms for sampling?

- PTIME => Polylog(n) rounds
- For parallel/distributed computing:
 sampling = approx counting/inference?
 - PTIME => Polylog(n) rounds
- Optimize of the state of the
 - $PTIME \implies Polylog(n)$ incremental cost

Graphical Model

 $\forall \sigma \in [q]^V : \quad \mu(\sigma) \propto \qquad \nu_v(\sigma_v) \qquad \phi_e(\sigma_e)$ $e \in E$ $v \in V$

- Each $v \in V$: a variable with domain [q] following distribution ν_v
- Each e∈E is a set of variables and corresponds to a constraint (factor)

 $\phi_e:[q]^e\to [0,1]$



Dynamic Sampling

• distribution μ over all $\sigma \in [q]^V$:

$$\mu(\sigma) \propto \prod_{v \in V} \nu_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e)$$

current sample: $X \sim \mu$

dynamic update:

- adding/deleting a constraint *e*
- changing a function v_v or ϕ_e
- adding/deleting an independent variable v

Question:

Obtain $X' \sim \mu$ ' from $X \sim \mu$ with small incremental cost.



Dynamic Sampling

Input: a graphical model which defines distribution μ a sample $X \sim \mu$, and an update changing μ to μ '

Output: a new sample $X' \sim \mu'$

- inference/learning tasks where the graphical model is changing dynamically
 - video processing
 - online learning with dynamic or streaming data
- sampling/inference/learning algorithms which adaptively and locally change the joint distribution
 - stochastic gradient descent
 - approximate counting / self-reduction

Dynamic Sampling

Input: a graphical model which defines distribution μ a sample $X \sim \mu$, and an update changing μ to μ '

Output: a new sample $X' \sim \mu'$

Goal:

transform a
$$X \sim \mu$$
 to a $X' \sim \mu'$ by local changes



Current sampling techniques are not powerful enough:

- μ could be changed significantly by dynamic updates;
- Monte Carlo sampling does not know when to stop;
- notions such as mixing time give worst-case estimation.

• distribution
$$\mu$$
 over all $\sigma \in [q]^{V}$:

$$\mu(\sigma) \propto \prod_{v \in V} \nu_{v}(\sigma_{v}) \prod_{e \in E} \phi_{e}(\sigma_{e})$$
distribution ν_{v} over $[q]$

$$\phi_{e} : [q]^{e} \rightarrow [0,1]$$

- each $v \in V$ independently samples $X_v \in [q]$ according to ν_v ;
- each $e \in E$ is passed independently with probability $\phi_e(X_e)$;
- X is accepted if all constraints $e \in E$ are passed.
- μ : distribution of X conditioning on accept
- Probability of accept is exponentially small!

For general graphical models:

Question I: (dynamic sampling)

Given a $X \sim \mu$, when $\mu \rightarrow \mu'$ transform X to a $X' \sim \mu'$.

Question II: (rejection sampling)

Make rejection sampling great again! (when part of X is rejected, only resample the rejected part while still being correct)

[Guo, Jerrum, Liu, STOC'17] for Boolean CSP

[Feng, Vishnoi, Y., STOC'19]

Dynamic Sampler

Upon receiving an update to the graphical model :

- Let *R* includes the variables affected by the update;
- while $R \neq \emptyset$:
 - $(X, R) \leftarrow \text{Resample}(X, R);$

Resample(X, R):

- each $e \in E^+(R)$ computes $\kappa_e = \min_{x_e: x_{e \cap R} = X_{e \cap R}} \phi_e(x_e) / \phi_e(X_e)$
- each $v \in R$ resamples $X_v \in [q]$ independently according to ϕ_v ;
- each $e \in E^+(R)$ is passed independently with prob. $\kappa_e \cdot \phi_e(X_e)$; (otherwise *e* is violated)
- $R \leftarrow \bigcup_{e \in E: \text{ violated } e} e^{e};$

Dynamic Sampler

[Feng, Vishnoi, Y., STOC'19]

Upon receiving an update to the graphical model :

- Let *R* includes the variables affected by the update;
- while $R \neq \emptyset$:
 - $(X, R) \leftarrow \text{Resample}(X, R);$

Resample(X, R):

- each $e \in E^+(R)$ computes $\kappa_e = \min_{x_e: x_{e \cap R} = X_{e \cap R}} \phi_e(x_e) / \phi_e(X_e)$
- each $v \in R$ resamples $X_v \in [q]$ independently according to ϕ_v ;
- each $e \in E^+(R)$ is passed independently with prob. $\kappa_e \cdot \phi_e(X_e)$; (otherwise *e* is violated)

•
$$R \leftarrow \bigcup_{e \in E: \text{ violated } e}^{e}$$

Correctness of Sampling

[Feng, Vishnoi, Y., STOC'19]

Upon receiving an update to the graphical model :

- Let *R* includes the variables affected by the update;
- while $R \neq \emptyset$:
 - $(X, R) \leftarrow \text{Resample}(X, R);$



Correctness:

Assuming input sample $X \sim \mu$, upon termination, the dynamic sampler returns a sample from the updated distribution μ '.

Correctness of Sampling

[Feng, Vishnoi, Y., **STOC**'19]

Upon receiving an update to the graphical model :

- Let *R* includes the variables affected by the update;
- while $R \neq \emptyset$:
 - $(X, R) \leftarrow \text{Resample}(X, R);$



Conditional Gibbs Property:

A random (X,R) is conditionally Gibbs w.r.t. μ if conditioning on any choice of R and X_R , the distribution of the rest $X_{V\setminus S}$, is correct.

Equilibrium:

If (X,R) is conditionally Gibbs w.r.t. μ ', then so is (X',R').

Fast Convergence

Upon receiving an update to the graphical model :

- Let R includes the variables affected by the update;
- while $R \neq \emptyset$:
 - $(X, R) \leftarrow \text{Resample}(X, R);$

Resample(X, R):

- each $e \in E^+(R)$ computes $\kappa_e = \min_{x_e: x_{e \cap R} = X_{e \cap R}} \phi_e(x_e) / \phi_e(X_e)$
- each $v \in R$ resamples $X_v \in [q]$ independently according to ϕ_v ;
- each e ∈ E⁺(R) is passed independently with prob. κ_e·φ_e(X_e); (otherwise e is violated)
 R ← ⋃_{e∈E} violated e^e;

Sufficient Condition for Fast Convergence:

If for the graphical model with max-edge-degree d:

$$\forall e \in E, \quad \min_{x} \phi_{e}(x) > \sqrt{1 - \frac{1}{d+1}}$$

then O(1) incremental cost per update in expectation.

- Las Vegas (good for simulation)
- parallel & distributed (good for systems)
- better static sampling algorithm

Parallel/distributed algorithms for sampling

- Feng, Sun, Y.: *What can be sampled locally?* **PODC**'17.
- Feng, Hayes, Y.: Distributed Sampling Almost-Uniform Graph Coloring with Fewer Colors. arXiv: 1802.06953.
- Feng, Hayes, Y.: Fully-Asynchronous Distributed Metropolis Sampler with Optimal Speedup. arXiv:1904.00943.
- For parallel/distributed computing: sampling = approx counting/inference

• Feng, Y.: On local distributed sampling and counting. **PODC**'18.

- Dynamic sampling algorithms
 - Feng, Vishnoi, Y.: *Dynamic Sampling from Graphical Models*. **STOC**'19.
 - Feng, He, Sun, Y.: *Dynamic MCMC Sampling*. arXiv:1904.11807.
 - Feng, Guo, Y.: Perfect sampling from spatial mixing. arXiv:1907.06033.

