

Randomness and Computation

or, “Randomized Algorithms”

Mary Cryan

School of Informatics
University of Edinburgh

Markov chain Monte Carlo

In Tuesday's slides, we assumed an "off the shelf" FPAUS for sampling independent sets of an input graph, and showed how to build an FPRAS for approximately counting ISs. The *Markov chain Monte Carlo method* is a common approach used to build the FPAUS.

In the Markov chain Monte Carlo method, the idea is to build a Markov chain M on the state space Ω that we want to sample from. Then we have to show the chain is ergodic (irreducible and aperiodic) and also have to verify that the unique stationary distribution π_M is the uniform distribution.

We can then run M to generate a sequence of $X_0, X_1, \dots, X_k, \dots$ of states (from some starting point X_0), and when X_k is "close enough" to the stationary distribution, return that as our sample.

Markov chain Monte Carlo (Independent Sets)

We describe an example Markov chain for *Independent Sets*. We have a given input graph $G = (V, E)$. Our interest is in sampling from the state space Ω containing all subsets $I \subseteq V$ which satisfy $|I \cap \{u, v\}| \leq 1$ for all u, v such that $e = (u, v) \in E$.

The IS Markov chain generates a random sequence of ISs:

Algorithm GENERATEIS($n; G = (V, E)$)

1. Start with an arbitrary IS X_0
2. **for** $i \leftarrow 0$ **to** "whenever"
3. Choose v uniformly at random from V .
4. **if** $v \in X_i$ **then**
5. $X_{i+1} \leftarrow X_i \setminus \{v\}$
6. **elseif** ($v \notin X_i$ **and** $X_i \cup \{v\}$ is also an IS in G) **then**
7. $X_{i+1} \leftarrow X_i \cup \{v\}$
8. **else** $X_{i+1} \leftarrow X_i$

Markov chain Monte Carlo (Independent Sets)

- ▶ Algorithm GENERATEIS describes how the Markov chain for ISs is used to generate a *sequence* of ISs of some (unspecified) length.
- ▶ The Markov chain itself $M_{IS} : \Omega \rightarrow \Omega$, is the process carried out in steps 3.-8..
- ▶ We would like to show the properties of *irreducibility* and *aperiodicity*. That will tell us that M_{IS} has a *unique* stationary distribution on Ω , π_{IS} say.
- ▶ After that we will want to show that this unique stationary distribution is the uniform one. That will tell us that *in the limit*, the chain settles down to a state *uniformly distributed* among all the elements of Ω .

In fact, having the uniform distribution as the unique stationary distribution does not give us an FPAUS for Ω . We need to also show the chain is *rapidly mixing*.

Markov chain Monte Carlo (Independent Sets)

We would like to show the properties of *irreducibility* and *aperiodicity*.

irreducible: Imagine we have two different ISs of G , let them be X and Y . We need to show we can connect them via a sequence of transitions of M_{IS} . Consider the vertices $X \setminus Y$ (in X but not in Y) and order these as $w_1, \dots, w_{|X \setminus Y|}$. Order the vertices $Y \setminus X$ (in Y but not in X) as $z_1, \dots, z_{|Y \setminus X|}$. Then we define the sequence

$$X = Z_0, Z_1, \dots, Z_{|X \setminus Y|}, Z_{|X \setminus Y|+1}, \dots, Z_{|X \oplus Y|} = Y$$

where $Z_j = X \setminus \{w_1, \dots, w_j\}$ for $j \leq |X \setminus Y|$, and $Z_j = Y \setminus \{z_{j-|X \setminus Y|}, \dots, z_{|Y \setminus X|}\}$ for $j, |X \setminus Y| < j \leq |X \oplus Y|$.

- ▶ We have $Z_j \subseteq X$ for $j \leq |X \setminus Y|$, so these are ISs.
- ▶ We have $Z_j \subseteq Y$ for $j \geq |X \setminus Y|$, so these are ISs.
- ▶ Each successive pair Z_j, Z_{j+1} differ by *one* vertex, so $M_{IS}[Z_j, Z_{j+1}] > 0$ (4-5, 6-7 of Alg GENERATEIS), as required.

Markov chain Monte Carlo (Independent Sets)

aperiodic: For this step we actually need one *tiny* assumption, which is that the graph contains *at least one edge* (very reasonable, since if not, we can easily sample as IS).

For any two ISs of G X and Y , we know we can connect them via a sequence of transitions of M_{IS} . We need to show that the *greatest common divisor* of the “path-lengths” of paths connecting X and Y is 1.

Let ℓ_{min} be the length of the path we used for irreducibility (the minimum-length path that could connect X to Y). We can “add and delete” any *addable* vertex to Z_j using an extra two steps, so $\ell_{min} + 2, \ell_{min} + 4$ etc are the lengths of possible X -to- Y paths.

However there is at least one edge in G , say (u, v) , and whenever Z contains one of $\{u, v\}$, there is a probability of $\geq \frac{1}{n}$ of “waiting at Z ”, hence $M[Z, Z] > 0$ for these Z s. Hence we have a path of length $\ell_{min} + 2k$ and also of $\ell_{min} + 2k + 1$, hence the gcd can only be 1.

Markov chain Monte Carlo (Independent Sets)

From the previous two slides, we know M_{IS} has a unique stationary distribution π_{IS} , but not what it *is*. We now show it must be the uniform one.

By definition ($\pi_{IS} \cdot M_{IS} = \pi_{IS}$), we have

$$\sum_{Y \in \Omega} \pi_{IS}(Y) M_{IS}[Y, X] = \pi_{IS}(X).$$

However, by lines 4,5 and 6,7 of our Markov chain, we know that $M_{IS}[Y, X] = M_{IS}[X, Y]$ for every $X, Y \in \Omega$. Hence, we can equivalently write,

$$\sum_{Y \in \Omega} \pi_{IS}(Y) M_{IS}[X, Y] = \pi_{IS}(X).$$

Now, if π_{IS} is uniform, then we have $\pi(Y) = \pi(X)$ for all Y , and hence

$$\sum_{Y \in \Omega} \pi_{IS}(Y) M_{IS}[X, Y] = \pi_{IS}(X) \cdot \sum_{Y \in \Omega} M_{IS}[X, Y].$$

By definition we always have $\sum_{Y \in \Omega} M_{IS}[X, Y] = 1$.

Hence for π_{IS} uniform we are asking whether $\pi_{IS}(X) \cdot 1 = \pi_{IS}(X)$ which of course is true.

Reading and Doing

Reading:

- ▶ These slides follow (some of) Section 11.4 from the book.
- ▶ You might want to read ahead to Sections 12.1 and 12.2.

Doing:

- ▶ Exercise 11.11 from the book (after reading all of 11.4).
- ▶ I will ship a tutorial sheet over the weekend (for our final tutorial in week 10).