An Introduction to Ensemble-Average Importance Sampling of Markov Chains

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Abstract

Using a simple Markov chain as an example, the paper introduces a new single-sample-path-based estimation method, the Ensemble-Average Importance Sampling (EAIS), and discusses its difference from the Likelihood Ratio (LR) method.

1. Introduction

In this paper, we introduce the idea of the EAIS method by applying it to a very simple Markov chain.

Consider a Markov chain \( X = \{X_1, X_2, ..., X_N\} \) with \( X_i \in \{1, 2, ..., M\} \). The state transition matrix of \( X \) is \( Q = \{q(i, j)\}_{i,j}^{M \times M} \). Let \( w(i) \) be the steady-state probability of state \( i \). Suppose that \( Q \) changes to \( Q' = \{q'(i, j)\}_{i,j}^{M \times M} \). Let \( w'(i) \) be the steady-state probability of the Markov chain with transition matrix \( Q' \).

The problem is, how do we estimate \( w'(i) \) by using sample paths of the Markov chain with \( Q' \)?

2. The Likelihood Ratio Method

Let \( I_i(X_n) = 1 \) for \( X_n = i \) and \( I_i(X_n) = 0 \) for \( X_n \neq i \), then by ergodicity of Markov chains,

\[
w(i) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} I_i(X_n) \quad \text{w.p.1.} \tag{1}
\]

We can use a finite \( N \) to obtain an estimate of \( w(i) \). (For \( M = 3 \), to get an estimate that is accurate to the third digit after the decimal point, at least \( N = 1000 \) is needed.)

The estimate based on the sample path \( X \) is

\[
w(i) \approx \frac{1}{L} \sum_{l=1}^{L} I_i(X_l) \tag{2}
\]

Given an initial state \( X_1 \), the probability of the sample path \( X \)

\[
P(X) = \prod_{n=1}^{N} p(X_n, X_{n+1}) \tag{3}
\]

The mean of the estimates is then

\[
E[I_X(i)] = \frac{1}{L} \sum_{l=1}^{L} I_i(X_l)P(X) \tag{4}
\]

which can be estimated by using an average as follows

\[
E[I_X(i)] \approx \frac{1}{L} \sum_{l=1}^{L} I_i(X_l) \tag{5}\]

where \( I_i(X_l) \), \( l = 1, 2, ..., L \), are the estimates obtained from \( L \) sample paths, \( X_l = \{X_1, X_2, ..., X_N\} \).

In the likelihood ratio (LR) method, we assume that the same sample paths are observed from the Markov chain with transition matrix \( Q' \). From (4), we have

\[
E[I_X(i)] \approx \frac{1}{L} \sum_{l=1}^{L} I_i(X_l)P'(X) \tag{6}
\]

where \( P'(X) \) is the probability that the sample path \( X \) occurs in the Markov chain with \( Q' \). From (6),

\[
E[I_X(i)] = \frac{1}{L} \sum_{l=1}^{L} I_i(X_l)P'(X) \tag{7}
\]

(7) can be estimated by the average

\[
E[I_X(i)] \approx \frac{1}{L} \sum_{l=1}^{L} I_i(X_l) \tag{8}
\]

where \( X_l = \{X_1, X_2, ..., X_N\} \), \( l = 1, 2, ..., L \), are sample paths of the Markov chain with \( Q' \).

(8) is called the LR estimate [4-6]; it usually has a large variance because the large value of \( N \). Regenerative structure is often used to reduce the variance.

3. The Ensemble-Average Importance Sampling (EAIS) method

We observe that in the LR method, the steady-state performance \( \bar{w}_X \) is estimated by an time average, which must be based on long sample paths in order to obtain certain accuracy. On the other hand, the sum in (8) represents, in fact, an ensemble average, which requires many sample paths to achieve a reasonable variance. In other
words, the LR estimate is an ensemble average of many long-time averages. The longer the time averages are, the smaller the bias of the time averages, but the larger the variance of the LR estimate.

Based on the above fundamental observations, the EAIS method is developed. In EAIS, we do not use time average to estimate the steady-state performance. Instead, we use an ensemble average to estimate the K-step transition matrix \( Q^k \), which is an approximation of \( \pi \). We then update \( \pi \) and use an ensemble average again to obtain an estimate of \( \pi' \).

Consider the Markov chain with transition matrix \( Q \). The conditional probability of \( X_{K+1} = j \), given that \( X_1 = i \) is the \((i,j)\)-entry of the \( K \)-step transition matrix \( Q^K \), i.e.,

\[
P(X_{K+1} = j| X_1 = i) = \sum_{X_1, \ldots, X_K \in \mathcal{X}} P(X_1, \ldots, X_{K+1}),
\]

with \( X_1 = i \) and \( X_K = j \). Assuming that the Markov chain is irreducible and aperiodic, we have

\[
\pi(j) = \lim_{K \to \infty} P(X_K = j| X_1 = i),
\]

independent of \( i \). We choose

\[
\theta(j) = P(X_{K+1} = j| X_1 = i)
\]

as the estimate of \( \pi(j) \). Since (10) converges much faster than the time average to the steady-state value, \( K \) can be much smaller than \( N \) in the LR method. (9) shows that \( \theta(j) \) can be estimated by an ensemble average. In fact, (9) has the same form as (8). Let \( X_1 = (X_1, \ldots, X_{K+1}) \), \( l = 1, 2, \ldots, L \), be \( L \) sample paths with \( X_1 = i \), \( X_{K+1} = j \). Then from (9), \( P(X_{K+1} = j| X_1 = i) \) can be estimated by

\[
P(X_{K+1} = j| X_1 = i) = \frac{1}{L} \sum_{l=1}^{L} P(X_{K+1} = j| X_1 = i)
\]

where \( (X_1, \ldots, X_{K+1}) \), \( l = 1, 2, \ldots, L \), are sample paths of the Markov chain with \( Q \). A comparison of the EAIS estimate (13) and the LR estimate (8) is straightforward. There are \( 2K \) transitions in (13), while in (8), \( (N - 1) L \) transitions. As we discussed, for \( M = 3, N = 1000 \), while \( K = 3 \) or even 2 is good enough. Also, it is easy to believe that (8) has a much bigger variance than (13).

In practice, it is convenient to use a single sample path to get the estimate. This can be done by dividing the long sample path into small segments, each of them consisting of \( K \) transitions. Thus, we obtain the following estimate of \( \pi'(j) \), which is based on a single sample path, \( (X_1, \ldots, X_{K+1}) \), of the Markov chain with transition matrix \( Q \).

\[
\pi'(j) = \frac{1}{D - K + 1} \sum_{d=0}^{D-K} \frac{1}{L} \sum_{l=1}^{L} \begin{cases} 1 & \text{if } X_{d+K+1} = j \\ 0 & \text{otherwise} \end{cases}
\]

An easily implementable algorithm for this estimate and the proof of its strong consistency can be found in [1]. As an example, we simulated a Markov chain with \( K = 3, D = 100,000 \), \( p(1,1) = 0.3, p(1,2) = 0.2, p(2,1) = 0.6, p(2,2) = 0.1, p(3,1) = 0.8, p(3,2) = 0.2 \). We obtain \( \theta'(1) = 0.165, \theta'(2) = 0.434, \theta'(3) = 0.401 \), while the theoretical values are \( \pi'(1) = 0.170, \pi'(2) = 0.426, \pi'(3) = 0.404 \).

Finally, let \( f(i) \) be a function on the state space. The steady-state performance value of the Markov chain with \( Q' \), \( f' = \sum_{i} f(i) \theta'(i) \), can also be estimated by simply replacing \( f(X_{K+1}) \) in (14) with \( f(X_{K+1}) \).

8. Conclusion

One of the intrinsic properties of the important sampling technique is that it uses ensemble averages. Applying it to time average values leads to inefficiency and large variance. Each long-time average provides only one sample point in the ensemble. The discussion in this note shows that applying important sampling to ensemble averages is desirable. In the EAIS method, \( \pi'(j) \) is first estimated by using an average over an ensemble of short sample paths. The sample points in the ensemble are then updated by a factor to obtain an estimate of \( \pi'(j) \).

The EAIS estimate is much more efficient than the time-average LR method and has less variance. It does not resort to regenerative structure.

The EAIS method has been applied to sensitivity analysis and has been extended to non-Markovian processes by using a uniformization technique (see [2]).

References

2. X. R. Cao, Sensitivity Analysis via Ensemble-Average Importance Sampling, manuscript, 1991b.
3. X. R. Cao, Uniformization and Discretization of the State Processes of Stochastic DBS, manuscript, 1991c.