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A SINGLE SAMPLE PATH-BASED PERFORMANCE SENSITIVITY FORMULA FOR MARKOV CHAINS

Xi-Ren Cao*, Xue-Ming Yuan†, Li Qiu

The Hong Kong University of Science and Technology
Clear Water Bay, Kowloon, Hong Kong

Abstract: With a sample path approach, a new formula is derived for performance sensitivities of discrete-time Markov chains. A distinguished feature of this formula is that the quantities involved can be estimated by analyzing a single sample path of a Markov chain. Thus, the formula creates a new direction for sensitivity analysis and can be viewed as an extension of the perturbation realization theory.

Keywords: Perturbation analysis, sensitivity analysis, Lyapunov equation, realization, performance evaluation.

1. INTRODUCTION

In this paper, a new formula is derived for performance sensitivities of discrete-time Markov chains (for simplicity, the term Markov chain is used hereafter). A sample-path approach is used, i.e., by a sample path, to determine the performance changes due to a change in the transition probability matrix. The formula shows that the derivative of a performance measure equals the weighted sum of the expected value of a quantity, called a *realization factor*, that measures the average performance change when the Markov chain changes from one state to another; the realization factors can be determined by solving a skew-symmetric Lyapunov equation. Furthermore, these realization factors can be estimated by analyzing a single sample path obtained from simulation or a record of a real system.

The formula provides a new perspective to the sensitivity analysis of Markov chains. It shows that a single sample path contains all the information needed for determining the performance sensitivities in a Markov chain. The approach can be viewed as an extension of the realization theory (Cao, 1987, 1994) in infinitesimal perturbation analysis (IPA) (Glasserman, 1991; Ho and Cao, 1991) to the case where a small change may induce a large change in the sample path. This work was motivated by a recent work of Dai and Ho (1994) and can be considered as a theoretical justification of the algorithm in Dai (1994).

The formula can be easily generalized to continuous-time Markov chains. Since Markov chain is the main

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model for many stochastic systems such as queueing systems, the formula developed here may have an impact in other fields, especially in the field of single-sample-path based sensitivity analysis and performance optimization.

The paper is organized as follows. Section 2 introduces the basic concepts derived from a sample path point of view. The simplest but the fundamental case is considered, where one transition probability increases and another transition probability decreases by the same amount. This section shows how the sensitivity formula can be derived by using intuition. Section 3 provides a rigorous proof for the general results where the transition matrix changes arbitrarily within the constraint of a stochastic matrix. The fundamental case discussed in Section 2 becomes a special case. Section 4 discusses the implication of the results.

2. THE BASIC CONCEPTS

In this section, the performance sensitivity formula is derived by using intuition. A sample-path argument is used. The basic concepts in this approach are introduced. The rigorous proof of the formula and other results will be provided in the next section.

Consider an irreducible and aperiodic Markov chain $X = \{X_n; n \geq 0\}$ on a finite state space $\mathcal{E} = \{1, 2, \cdots, M\}$ with transition probability matrix $P = [p_{ij}]_{i=1}^{M}|_{j=1}^{M}$. The Markov chain is defined on a probability space $(\Omega, \mathcal{F}, \mathcal{P})$.

A Markov chain is said to be reducible, if by renumbering the states of the Markov chain, P can be rewritten as the following form:

$$\begin{pmatrix} P_1 & Q \\ O & P_2 \end{pmatrix},$$

with O denoting a matrix whose elements are all zeros. If $Q = O$, then the Markov chain can be decomposed into two (or more, if P_1 and P_2 are further reducible) small independent Markov chains with P_1 and P_1 as their transition matrices. If $Q \neq 0$, then in steady-state, the Markov chain cannot visit the states corresponding to P_1, and the Markov chain is equivalent to a sub-Markov chain with transition matrix P_2. Thus, the condition "irreducible" is not restrictive. Next, if an irreducible Markov chain is periodic, then all the states have the same period (Çinlar, 1971). However, if $p_{ii} \neq 0$ for some i, then i is not periodic. Therefore, a Markov chain is aperiodic if $p_{ii} \neq 0$ for some i. For practical systems modeled by continuous-time Markov chains, it is easy to obtain an embedded Markov chain with $p_{ii} \neq 0$, by simply increasing the rate of sampling at state i. Therefore, the condition "aperiodic" is also not restrictive in practice.

Let $f : \mathcal{E} \to \mathcal{R}$, where $\mathcal{R} := (-\infty, \infty)$ represents the space of real numbers, and $\pi = (\pi_1, \pi_2, \cdots, \pi_M)$ be the vector representing the steady-state probability of $\{X_n;\ n \geq 0\}$. f is called a *performance function*. The performance measure is defined as its expected value with respect to π:

$$\eta = E(f) = \sum_{i=1}^{M} \pi_i f(i) = \pi f, \tag{1}$$

where $f = (f(1), f(2), \cdots, f(M))^T$ is a column vector, and E denotes the expectation with respect to the steady state measure π.

Assume that the transition matrix P is perturbed to $P' = [p'_{ij}]_{i=1}^{M}|_{j=1}^{M}$. In this section, the most fundamental case is considered, where

$$p'_{ij} = \begin{cases} p_{ls} - \delta, & i = l,\ j = s; \\ p_{lt} + \delta, & i = l,\ j = t; \\ p_{ij}, & \text{otherwise}, \end{cases} \tag{2}$$

for some arbitrarily fixed $l, s, t \in \mathcal{E}$, and any small real number $\delta \in (0, p_{ls}]$. The Markov chain with transition matrix P' is denoted as $X' = \{X'_n;\ n \geq 0\}$. Let $\pi' = (\pi'_1, \pi'_2, \cdots, \pi'_M)$ be the steady state probability of X'. The performance measure of X' is

$$\eta' = \sum_{i=1}^{M} \pi'_i f(i) = \pi' f.$$

The derivative of η with respect to δ is defined as

$$\frac{\partial \eta}{\partial \delta} = \lim_{\delta \to 0} \frac{\eta' - \eta}{\delta}. \tag{3}$$

Of course, this derivative can be obtained via $\frac{\partial \pi}{\partial \delta}$. Our purpose is to derive another formula for $\frac{\partial \eta}{\partial \delta}$ based on a sample-path approach.

Consider a sample path of X with a finite length, $\{X_n; 0 \leq n < L\}$, and define a *sample performance measure*

$$\eta_L = \frac{1}{L} \sum_{n=0}^{L-1} f(X_n). \tag{4}$$

Since X is irreducible, aperiodic and finite, it is ergodic (Çinlar, 1971). Thus,

$$\eta = \lim_{L \to \infty} \eta_L \qquad a.s.$$

That is, η can be approximated by η_L provided L is large enough.

In simulation, X can be generated as follows. Let $\xi_0, \xi_1, \cdots, \xi_n, \cdots$ be a sequence of independent random variables, each of them is uniformly distributed on $[0, 1)$. Given an $X_n = i$, $n = 0, 1, 2, \cdots$, assign $X_{n+1} = j$, $j = 1, 2, \cdots, M$, if

$$\sum_{k=1}^{j-1} p_{ik} \le \xi_n < \sum_{k=1}^{j} p_{ik}, \tag{5}$$

(by convention, $\sum_{k=1}^{0} p_{ik} = 0$). In this setting, the probability space is $\Omega = [0, 1)^L$, $\mathcal{F}$ is the Borel field on the hypercube, and $\mathcal{P}$ is the Lebesgue measure.

Suppose P changes to P'. Let us evaluate the effect of such a change on a sample path. Assume that because of the change the sample path $\{X_n; 0 \le n < L\}$ changes to $\{X'_n; 0 \le n < L\}$. To estimate the performance change, the same sequence $\xi_0, \xi_1, \cdots, \xi_n, \cdots$ may be used to generate X'. This corresponds to the simulation technique of "common random numbers" in estimating the difference of two random variables (Bratley, *et al.*, 1982). P' differs from P by only two terms: p'_{ls} and p'_{lt}. Therefore, the state transition of X' can be determined by matrix P and (5) with a slight modification. Specifically, if ξ_n satisfies (5) with $i \ne l$ or $j \ne s$, then $X'_{n+1} = j$ (no changes). When $i = l$ and $j = s$, the transition scheme is modified:

1. if $\sum_{k=1}^{s-1} p_{lk} \le \xi_n < \sum_{k=1}^{s} p_{lk} - \delta = \sum_{k=1}^{s} p'_{l,k}$, then $X'_{n+1} = s$;
2. if $\sum_{k=1}^{s} p_{lk} - \delta \le \xi_n < \sum_{k=1}^{s} p_{lk}$, then $X'_{n+1} = t$.

In words, this means moving a portion of δ from state s to state t. Obviously, the transitions thus generated are consistent with the transition matrix P'.

From the above discussion, the state transition may change only when the Markov chain is at state l. Because $p'_{ls} = p_{ls} - \delta$ and $p'_{lt} = p_{lt} + \delta$, some transitions in X from l to s may become transitions in X' from l to t. It is obviously that when X is at state l, the probability of such transition changes is δ.

Starting from the same initial state, X and X' will be the same in an initial period; the two sample paths may differ only after the Markov chains reach state l at some time k, i.e., $X_k = l$ and $X'_k = l$; at time $k+1$, it happens that $X_{k+1} = s$ and $X'_{k+1} = t$.

The effect of a state changing from s to t on a sample performance measure can be visualized as follows. For simplicity, renumber the time indexes such that $k + 1 = 0$, and run the two Markov chains X and X' with $X_0 = s$ and $X'_0 = t$ with the same sequence of random numbers. Let

$$F_L = \sum_{n=0}^{L} f(X_n).$$

The effect of the change from $X_0 = s$ to $X'_0 = t$ on the sample performance measure is reflected by

$$\Delta F_L = \sum_{n=0}^{L} [f(X'_n) - f(X_n)]$$

with $X_0 = s$ and $X'_0 = t$.

Its expected value is denoted as

$$d'_{st} = E(\sum_{n=0}^{L} [f(X'_n) - f(X_n)] | X_0 = s, X'_0 = t), \tag{6}$$

where L is considered as a very large number, X evolves according to P and X' evolves according to P'. It is easy to see that at some point $n = L^*$, X'_n and X_n may reach the same state, i.e., $X_{L^*} = X'_{L^*}$. After this point X'_n and X_n will behave statistically similarly. Therefore, L in (6) can be replaced by L^*, i.e.,

$$d'_{st} = E(\sum_{n=0}^{L^*} [f(X'_n) - f(X_n)] | X_0 = s, X'_0 = t).$$

Thus, the effect of the change from $X_0 = s$ to $X'_0 = t$ on performance terminates when the chain reaches L^*.

With the above observations, the formula for the derivative can be devised. Among the L transitions on a sample path $\{X_n; L > n \ge 0\}$, the Markov chain X visits state l, on the average, $L\pi_l$ times. Because the probability that a transition from l to s changes to a transition from l to t is δ, on the sample path there are, on the average, $L\pi_l\delta$ times when state s changes to state t. Each time the state changes from s to t, F_L changes, on the average, by the amount d'_{st}. In addition, because δ can be chosen arbitrarily small and L^* is always finite, the probability of two changes from s to t occurring within L^* state transitions is of order δ^2 and is hence negligible. This implies that the effect of each change can be treated separately. Therefore, the total change of η due to the change of P is

$$\Delta\eta = \frac{1}{L}\Delta F_L = \frac{1}{L}\{L\pi_l\delta d'_{st}\} = \pi_l\delta d'_{st}.$$

Finally,

$$\frac{\partial\eta}{\partial\delta} = \lim_{\delta\to 0}\frac{\eta' - \eta}{\delta} = \pi_l d_{st}. \tag{7}$$

In (7),

$$d_{st} = E(\sum_{n=0}^{L^*}[f(X_n') - f(X_n)]|X_0 = s, X_0' = t), \quad (8)$$

where both X and X' evolve according to P.

The new formula (7) is obtained by using a sample path argument. A mathematical proof of the formula and the equations determining d_{ij}, $i, j \in \mathcal{E}$, will be provided in the next section. The explanation in this section shows that the sample path approach may lead to new perspectives as well as new results. The theory is a counterpart of the realization theory in perturbation analysis (Cao, 1994; Ho and Cao, 1991) in the case where there are finite changes in sample paths.

3. THE MAIN RESULTS

In this section, the performance sensitivity formula will be rigorously established for the general case where the transition matrix changes arbitrarily within the constraint of a stochastic matrix.

3.1. The Realization Matrix

Consider an irreducible aperiodic Markov chain X, with a transition matrix P and state space $\mathcal{E} = \{1, 2, \cdots, M\}$. Let X' be another Markov chain, independent of X, with the same state space $\mathcal{E}$ and the same transition matrix P. Assume that the initial states of both chains may be different, $X_0 = i$, $X_0' = j$, with $i, j \in \mathcal{E}$.

Define $Y_n = (X_n, X_n')$, $n = 0, 1, \cdots$. Then $Y = \{Y_0, Y_1, \cdots, Y_n, \cdots\}$ is a Markov chain with state space $\mathcal{E} \times \mathcal{E}$ and transition matrix $P \otimes P$ (the Kronecker product).

Lemma 1 *Y is irreducible and aperiodic, hence all the states of Y are recurrent non-null. That is, the first arrive time from any state to any other state has a finite mean.*

Proof: For irreducibility, it suffices to prove that the Markov chain Y can reach any state $(k, l) \in \mathcal{E} \times \mathcal{E}$ from any other state $(i, j) \in \mathcal{E} \times \mathcal{E}$ with a positive probability. This is, however, obvious. In fact, since X is irreducible, the probability that X reaches k from i in h_1 steps, α, is positive; similarly, the probability that X' reaches l from j in h_2 steps, β is also positive. Because X and X' are independent, the probability that the Markov chain Y reaches (k, l) from (i, j) in $h_1 h_2$ steps is $\alpha^{h_2}\beta^{h_1} > 0$. Therefore, the Markov chain Y is irreducible. It is aperiodic since X and X' are. Since $\mathcal{E} \times \mathcal{E}$ is finite, all the states are recurrent non-null (Çinlar, 1971).

Let $\mathcal{S} = \{(k, k) : k \in \mathcal{E}\}$. Let L^* be the random variable such that at $n = L^*$, Y reaches $\mathcal{S}$ for the first time. From Lemma 1, $E(L^*)$ is finite.

Definition 1 *For $f : \mathcal{E} \to \mathcal{R}$, $d_{ij} = E\{\sum_{n=0}^{L^*}[f(X_n') - f(X_n)]|X_0 = i, X_0' = j\}$, $i, j = 1, 2, \cdots, M$, is called a perturbation realization factor; the matrix $D = [d_{ij}]$ is called a realization matrix.*

The meaning of the perturbation realization factor is as follows: Suppose that a Markov chain is perturbed by some reason such that the state changes from i to j. This perturbation will affect the system performance. The effect can be expressed as

$$\begin{aligned} & E\{\sum_{n=0}^{\infty}[f(X_n') - f(X_n)]|X_0 = i, \ X_0' = j\} \\ = \ & E\{\sum_{n=0}^{L^*}[f(X_n') - f(X_n)]|X_0 = i, \ X_0' = j\} \\ + \ & E\{\sum_{n=L^*+1}^{\infty}[f(X_n') - f(X_n)]|X_{L^*} = X_{L^*}'\}. \end{aligned}$$

The second term is zero. Therefore, d_{ij} measures the average effect of this perturbation on the performance measure. This is in parallel to the theory for IPA (Cao, 1987, 1994). The perturbation from i to j is *realized* at L^* on the sample path.

By definition, $d_{ji} = -d_{ij}$. That is,

$$D^T = -D.$$

Denote

$$F = ef^T - fe^T$$

where $e = (1, 1, \cdots, 1)^T$, and define two subspaces of $\mathcal{R}^{M \times M}$:

$$\begin{aligned} \mathcal{U} &= \{X \in \mathcal{R}^{M \times M} : X^T = -X\} \\ \mathcal{V} &= \{ex^T - xe^T : x \in \mathcal{R}^M\}. \end{aligned}$$

Clearly, $\mathcal{V} \subset \mathcal{U}$, $D \in \mathcal{U}$, and $F \in \mathcal{V}$.

Theorem 1 *The realization matrix D is the unique solution in $\mathcal{U}$ of the Lyapunov equation*

$$D - PDP^T = F. \quad (9)$$

Furthermore, $D \in \mathcal{V}$.

Proof: First let us prove that D satisfies (9). For any $i, j \in \mathcal{E}$,

$$\begin{aligned} d_{ij} &= E(\sum_{n=0}^{L^*}[f(X'_n) - f(X_n)]|X_0 = i, X'_0 = j) \\ &= f(j) - f(i) + \\ &\quad \sum_{i'=1}^{M}\sum_{j'=1}^{M} E(\sum_{n=1}^{L^*}[f(X'_n) - f(X_n)]| \\ &\qquad X_1 = i', X'_1 = j') \\ &\quad \cdot P\{X_1 = i', X'_1 = j'|X_0 = i, X'_0 = j\} \\ &= f(j) - f(i) + \sum_{i'=1}^{M}\sum_{j'=1}^{M} p_{ii'}p_{jj'}d_{i'j'}. \end{aligned}$$

By writing the above equations in matrix form, (9) holds.

Consider now the Lyapunov map $\boldsymbol{L}$:

$$\mathcal{R}^{M\times M} \to \mathcal{R}^{M\times M},$$

defined by

$$\boldsymbol{L}(D) = D - PDP^T.$$

Simple algebra shows that $\mathcal{U}$ is an invariant subspace of $\boldsymbol{L}$. It is well known (Marcus, 1973) that the restriction of $\boldsymbol{L}$ in $\mathcal{U}$ has eigenvalues $1 - \lambda_i(P)\lambda_j(P)$, $1 \le i < j \le n$, where $\lambda_i(P)$ denotes the i-th eigenvalue of P. Because X is irreducible and aperiodic, P is primitive; it follows that 1 is the only eigenvalue of P with maximum modulus. Hence this restriction is invertible, which means that for each $F \in \mathcal{U}$, there is a unique $D \in \mathcal{U}$ such that (9) is satisfied. Since $\mathcal{V}$ is also an invariant subspace of $\boldsymbol{L}$ and the restriction of $\boldsymbol{L}$ to $\mathcal{U}$ is invertible, it follows that the resriction of $\boldsymbol{L}$ to $\mathcal{V}$ is also invertible, which implies that $D \in \mathcal{V}$ for each $F \in \mathcal{V}$.

$D \in \mathcal{V}$ implies

$$d_{ik} = d_{ij} + d_{jk}, \qquad \textit{for all } i, j, k. \tag{10}$$

Corollary 1 *The unique skew-symmetric solution to (9) is given by*

$$D = \sum_{n=0}^{\infty} P^n F (P^T)^n.$$

Proof: By replacing the D on the right-hand side of (9) by $F + PDP^T$ and working iteratively, it follows

$$D = \sum_{n=0}^{N} P^n F (P^T)^n + P^{N+1} D (P^T)^{N+1}. \tag{11}$$

Since X is irreducible and aperiodic, there is (Çinlar, 1971)

$$\lim_{N\to\infty} P^N = e\pi.$$

Because $D^T = -D$, $(\pi D \pi^T)^T = -\pi D \pi^T = 0$. Therefore,

$$\lim_{N\to\infty} P^N D (P^T)^N = e\pi D \pi^T e^T = 0.$$

The corollary follows directly from this and (11).

3.2. The Derivative Formula

Now assume that P is perturbed to P' according to the following pattern:

$$P' = P + \delta Q \tag{12}$$

where $\delta > 0$ is a small real number and $Qe = 0$.

Let π and π' be the steady-state probabilities of the Markov chain with P and P', and $\eta = \pi f$ and $\eta' = \pi' f$ be their steady state performance measures respectively. The performance derivative of η is defined as

$$\frac{\partial \eta}{\partial \delta} = \lim_{\delta\to 0}\frac{\eta' - \eta}{\delta}.$$

The derivatives of other quantities are defined in a similar way.

Lemma 2 $\frac{\partial \pi}{\partial \delta} = \pi Q (I - P + e\pi)^{-1}$.

Proof: By taking derivatives of the both sides of $\pi P = \pi$ with respect to δ, it follows

$$\frac{\partial \pi}{\partial \delta}(I - P) = \pi \frac{\partial P}{\partial \delta} = \pi Q.$$

By using $\frac{\partial \pi}{\partial \delta} e = 0$, it follows

$$\frac{\partial \pi}{\partial \delta}(I - P + e\pi) = \pi Q,$$

where $I - P + e\pi$ is called the *fundamental matrix* (Kemeny and Snell, 1960) and is invertible. The lemma then follows immediately (see also Dai (1994)).

Theorem 2 $\frac{\partial \eta}{\partial \delta} = \pi Q D^T \pi^T$.

Proof: From Lemma 2,

$$\begin{aligned} \frac{\partial \eta}{\partial \delta} &= \frac{\partial \pi}{\partial \delta} f \\ &= \pi Q (I - P + e\pi)^{-1} f. \end{aligned} \tag{13}$$

Since $D = F + PDP^T$, $\pi e = 1$, and $\pi P = \pi$,

$$\begin{aligned} D^T \pi^T &= F^T \pi^T + PD^T P^T \pi^T \\ &= f - (\pi f) e + PD^T \pi^T. \end{aligned}$$

Furthermore,

$$(I - P + e\pi) D^T \pi^T = (\pi D^T \pi^T) e + f - (\pi f) e.$$

Thus,

$$\begin{aligned} &(I - P + e\pi)^{-1} f \\ &= D^T \pi^T + (\pi f - \pi D^T \pi^T)(I - P + e\pi)^{-1} e \\ &= D^T \pi^T + (\pi f - \pi D^T \pi^T) e. \end{aligned}$$

The last equation is due to $(I - P + e\pi)e = e$. Therefore, from (13) and $Qe = 0$,

$$\begin{aligned} \frac{\partial \eta}{\partial \delta} &= \pi Q \left[D^T \pi^T + (\pi f - \pi D^T \pi^T) e \right] \\ &= \pi Q D^T \pi^T. \end{aligned}$$

For the case discussed in Section 2, $q_{ts} = -1$, $q_{tt} = 1$ and $q_{ij} = 0$ for $i \neq t$ or $j \neq t, s$. There is

$$\begin{aligned} \frac{\partial \eta}{\partial \delta} &= \pi_t \sum_{j=1}^{M} \sum_{k=1}^{M} \pi_j q_{tk} d_{jk} \\ &= \pi_t \sum_{j=1}^{M} \pi_j (q_{ts} d_{js} + q_{tt} d_{jt}) \\ &= \pi_t \sum_{j=1}^{M} \pi_j (d_{jt} - d_{js}) \\ &= \pi_t d_{st}. \end{aligned} \qquad (14)$$

The last equation is due to (10). Thus, $\frac{\partial \eta}{\partial \delta}$ equals the expected value of d_{st}.

4. DISCUSSIONS

With a sample path approach, a new formula has been derived for the performance sensitivity of Markov chains. A distinguished feature of this formula is that the quantities involved can be estimated by analyzing a single sample path of a Markov chain.

To estimate d_{st} defined in (8) on a sample path of a Markov chain X, one may proceed as follows. First, find an $X_i = s$ and an $X_j = t$ on the sample path. Then record $\sum_{n=i}^{i+L} f(X_n)$ and $\sum_{n=j}^{j+L} f(X_n)$ until $X_{i+L} = X_{j+L}$. The average of $\sum_{n=i}^{i+L} f(X_n) - \sum_{n=j}^{j+L} f(X_n)$ is an ...timate of d_{st}. This demonstrates the important principle that a single sample path contains all information of performance sensitivity.

Dai (1994) proposed a simulation algorithm which in fact estimates the realization factors. In Dai's method, an additional simulation for a Markov chain X' with the initial state t is carried out when X reaches s. The additional simulation stops when X' and X reach the same state. The results obtained in this paper thus provide a clear interpretation of Dai's method as well as a rigorous proof of the algorithm in Dai (1994).

To develop single sample path-based algorithms using the formula for estimating performance sensitivities of practical systems is an on-going research topic.

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