ON THE OPTIMAL TRANSITION MATRIX FOR MCMC SAMPLING

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Abstract: Let $\mathcal{X}$ be a finite space and π be an underlying probability on $\mathcal{X}$. For any real-valued function f defined on $\mathcal{X}$, we are interested in calculating the expectation of f under π. Let $X_0, X_1, \ldots, X_n, \ldots$ be a Markov chain generated by some transition matrix P with invariant distribution π. The time average, $\frac{1}{n}\sum_{k=0}^{n-1} f(X_k)$, is a reasonable approximation to the expectation, $E_\pi[f(X)]$. Which matrix P minimizes the asymptotic variance of $\frac{1}{n}\sum_{k=0}^{n-1} f(X_k)$? The answer depends on f. Rather than a worst-case analysis, we will identify the set of P's that minimize the average asymptotic variance, averaged with respect to a uniform distribution on f.

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