Commun. Math. Phys. 115, 553–569 (1988)

Communications in
Mathematical
Physics

Simulated Annealing via Sobolev Inequalities

Richard Holley[1]* and Daniel Stroock[2]**

[1] Department of Mathematics, University of Colorado, Boulder, Colorado 80309–0426, USA
[2] Department of Mathematics, M.I.T., Cambridge, MA 02139, USA

Abstract. We use Sobolev inequalities to study the simulated annealing algorithm. This approach takes advantage of the local time reversibility of the process and yields the optimal "freezing schedule" as well as quantitative information about the rate at which the process is tending to its ground state.

0. Introduction

Simulated annealing is a Monte Carlo method for locating the minimum of a complicated function U on some space $\mathbf{E}$. Thinking of $U(x)$ as the "energy" of the "state" $x \in \mathbf{E}$, the method is to run a time-inhomogeneous Markov process on $\mathbf{E}$ in such a way that at any time $t \geqq 0$ the corresponding instantaneous time-homogenous Markov process has as its equilibrium distribution the Gibbs measure with energy U at inverse temperature $\beta(t)$. By choosing $t \to \beta(t)$ to go to infinity as $t \to \infty$, the idea is to force the process toward the minima of U.

Inherent in the simulated annealing procedure is a competition between two goals. On the one hand, one wants to make the temperature tend to 0 as fast as possible, thereby concentrating the Gibbs measures as fast as possible near the minima of U. On the other hand, having the Gibbs measure concentrated near the minima of U will do one no good unless the process at large times is close to equilibrium. Since, as we will see below (cf. Theorem (2.1)), decreasing the temperature inhibits equilibration, one must be careful not to adopt too fast a "freezing schedule" (i.e. rate at which $\beta(t) \to \infty$).

The problem raised above has been studied previously by many authors ([1–7]), and much of what we prove below is qualitatively similar to known results. Nonetheless, we believe that our approach to this problem has several features to recommend it. In the first place, it is simple and essentially context independent. Secondly, it yields quantitative information about the rate at which the process is tending to the minima of U. In fact, the results in Sect. 2 indicate

* Research supported in part by NSF Grant DMS-8609944
**Research supported in part by NSF Grant DMS-8611487 and ARO DAAL03-86-K-0171