OPTIMAL ACCEPTANCE PROBABILITY FOR SIMULATED ANNEALING

GEORGE KESIDIS and EUGENE WONG

University of California at Berkeley, Berkeley, CA 94720, USA

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The objective of this note is two-fold: first, to prescribe a rather general form for the acceptance probability which will attain the Gibbs distribution for a stationary Markov chain; second, to find the particular one that will maximize the rate at which equilibrium is reached.

KEY WORDS: Gibbs field, Markov chain, Boltzmann machine, simulated annealing.

1. INTRODUCTION

Let \( S \) be a finite set and let \( \mu \) be a probability measure on \( S \) such that \( \mu(x) > 0 \) for every \( x \). We define a Gibbs field as a Markov chain \( \{ X_t, t = 0, 1, 2, \ldots \} \) with values in \( S \) and with its equilibrium distribution given by the Gibbs distribution

\[
P_0(x) = \frac{1}{Z(T)} e^{-\frac{1}{T}U(x)} \mu(x)
\]  

(1.1)

where we interpret \( T \) as the temperature, \( U(x) \) as an energy function, and

\[
Z(T) = \sum_x e^{-\frac{1}{T}U(x)} \mu(x)
\]  

(1.2)

is known as the partition function.

To get (1.1), one can choose the transition probability

\[
P(x'|x) = \text{Prob}(X_{t+1} = x'|X_t = x)
\]  

(1.3)

with considerable latitude. The objective of this note is two-fold: first, to prescribe a rather general family of \( P(x'|x) \) that will result in (1.1); second, to find the one that optimizes (in a suitable sense) the rate at which the equilibrium distribution (1.1) is reached.

This problem is of considerable interest in simulated annealing (Holley and Stroock [3], Aarts and Jorst [1]) which is a stochastic algorithm for finding the
minimum of the function $U(x)$. There, a Gibbs field in equilibrium is “cooled” by letting $T$ be replaced by a function $T(t)$ that decreases to 0 as $t \to \infty$. The cooling must be sufficiently slow so that “quasi-equilibrium” is maintained. Intuitively, this means that the more quickly equilibrium is restored as temperature changes, the more quickly annealing can be achieved.

2. A GENERAL FORM FOR THE ACCEPTANCE PROBABILITY

The transition probability $P(x'|x)$ for a Gibbs field can be chosen as follows: Given $X_i = x$, we first choose a point $y \in S$ according to a probability $q(x, y)$, and set:

$$x_{i+1} = y \quad \text{with probability } p(\Delta U)$$

$$= x \quad \text{with probability } 1 - p(\Delta U)$$

where $\Delta U = U(y) - U(x)$. We call $p(\Delta U)$ the acceptance probability. It follows that

$$P(y|x) = q(x, y)p(U(y) - U(x)) \quad y \neq x$$

and

$$P(x|x) = 1 - \sum_{x \neq x} q(x, x')p(U(x') - U(x)). \quad (2.1)$$

The conventional choice for the acceptance probability is

$$p(\Delta U) = \min(1, e^{-(1/T)\Delta U}) \quad (2.2)$$

and an alternative choice is

$$p(\Delta U) = (1 + e^{(1/T)\Delta U})^{-1}. \quad (2.3)$$

The first corresponds to the so-called heat-bath model and the second to the Metropolis algorithm (Metropolis et al. [4]). If $q$ is $\mu$ symmetric and irreducible then either of these choices will yield the desired Gibbs distribution (1.1) for the stationary distribution. Our first result is to give a general form for the acceptance probability to achieve (1.1), a form that includes both (2.2) and (2.3) as special cases.

**Theorem 1** Let $q$ be $\mu$-symmetric, i.e.,

$$\mu(x)q(x, y) = \mu(y)q(y, x) \quad (2.4)$$

and irreducible, i.e.,
\[
\sum_{n=0}^{\infty} q^{(n)}(x, y) = \infty \quad \text{for all } x, y \in S
\]

where

\[
q^{(n+1)}(x, y) = \sum_{x' \in X} q(x, x') q^{(n)}(x', y).
\]

Let the transition probability be determined by (2.1). Then, the equilibrium distribution is given by (1.1) if the acceptance probability has the form

\[
p(\Delta U) = e^{-(1/2T)\Delta U} g(\Delta U), \quad \Delta U \in (-\infty, \infty).
\]  

(2.5)

Proof With \( P_0(x) \) given by (1.1) and with the use of (2.5) in (2.1), we get

\[
P(y|x)P_0(x) = \mu(x)q(x, y)g(\Delta U)1/Z e^{-(1/2T)[U(x) + U(y)]}.
\]

It then follows from (2.4) that

\[
P(y|x)P_0(x) = P(x|y)P_0(y)
\]

and

\[
\sum_x P(y|x)P_0(x) = P_0(y)
\]

so that \( P_0 \) is a stationary distribution. Irreducibility then ensures that \( P_0 \) is also the equilibrium distribution, i.e. (Feller [2])

\[
P_n(y|x) = \text{Prob}(X_{t+n} = y | X_t = x) \xrightarrow{n \to \infty} P_0(y). \quad \text{Q.E.D.}
\]

We note that the two choices of acceptance probability given by (2.2) and (2.3) can be put into the form (2.5) as follows:

\[
p(v) = \min(1, e^{-(1/T)\Delta U}) = e^{-(1/2T)\Delta U} e^{-(1/2T)\Delta U}
\]  

(2.6)

\[
p(v) = (1 + e^{(1/T)\Delta U})^{-1} = e^{-(1/2T)\Delta U} \left( 2 \cosh \frac{\Delta U}{2T} \right)^{-1}.
\]  

(2.7)

3. CONVERGENCE TO EQUILIBRIUM

The rate of convergence to equilibrium can be estimated by considering the following eigenvalue problem:

\[
\sum_x P(y|x)P_0(x)\theta(x) = \lambda P_0(y)\theta(y), \quad y \in S.
\]  

(3.1)
With (2.4) and (2.5), we have
\[ P(y|x)P_0(x) = P(x|y)P_0(y) \]
and there exist orthonormal eigenfunction \( \theta_v(x) \), \( v = 0, 1, 2, \ldots, N \), such that
\[ P_*(y|x) = P_0(y) \sum_{v=0}^{N} \lambda_v^* \theta_v(y) \theta_v(x). \]
The eigenvalues can be ordered so that
\[ \lambda_0 = 1 > \lambda_1 \geq \lambda_2 \geq \cdots \]
and \( \theta_0(x) \equiv 1 \). Since
\[ |P_*(y|x) - P_0(y)| = P_0(y) \left| \sum_{v=1}^{N} \lambda_v^* \theta_v(y) \theta_v(x) \right| \]
\[ = \lambda_1 \left| P_0(y) \sum_{v=1}^{N} \left( \frac{\lambda_v^*}{\lambda_1^*} \right)^n \theta_v(y) \theta_v(x) \right| \leq K \lambda_1^* \]
the second largest eigenvalue \( \lambda_1 \) provides an estimate of the rate of convergence. Our objective is to find the particular choice of \( g(\cdot) \) in (2.5) that would minimize \( \lambda_1 \).

**Theorem 2** Under the condition of Theorem 1, the eigenvalue \( \lambda_1 \) is minimized by the choice
\[ g_0(v) = e^{-1/2T} v. \]

**Proof** We can write
\[ \lambda_1 = \max_{\theta} \left[ \sum_{y,x} P(y|x)P_0(x)\theta(x)\theta(y) \right] \tag{3.3} \]
subject to
\[ \sum_x P_0(x)\theta(x) = 0 \tag{3.4a} \]
and
\[ \sum_x P_0(x)\theta^2(x) = 1. \tag{3.4b} \]
With (2.1) and (2.4), we can rewrite (3.3) as

$$
\lambda_1 = \max_\theta \left\{ \sum_y \sum_x P(y|x) P_o(x) \theta(x) \theta(y) + \sum_y P(y|y) P_o(y) \theta^2(y) \right\} 
$$

$$
= 1 + \max_\theta \left\{ \sum_y \sum_x \alpha(x, y) g(|U(x) - U(y)|) [\theta(y) \theta(x) - \theta^2(y)] \right\} 
$$

where

$$
\alpha(x, y) = \mu(x) q(x \cdot y) e^{-(1/2)T(|U(x) + U(y)|)} 
$$

and we have used (3.4b) and the symmetry of $\alpha(\cdot)$.

Since the sum in (3.5) is symmetric in $x$ and $y$, we must have

$$
\lambda_1 = 1 + \max_\theta \left\{ \frac{1}{2} \sum_{x,y} \alpha(x, y) g(|U(x) - U(y)|) \cdot [2\theta(y) \theta(x) - \theta^2(x) - \theta^2(y)] \right\} 
$$

$$
= 1 - \frac{1}{2} \min_\theta \sum_{x,y} \alpha(x, y) g(|U(x) - U(y)|) [\theta(x) - \theta(y)]^2 
$$

(3.6)

subject to the constraints in (3.4). Now, the function $g(\cdot)$ is related to the acceptance probability through (2.5). It follows that

$$
p(u) = e^{-(1/2)T} e^{u g(|u|)} \leq 1, \quad u \in (-\infty, \infty). 
$$

Hence,

$$
g(|u|) \leq e^{(1/2)T u}, \quad -\infty < u < \infty. 
$$

Taking $u$ to be negative yields

$$
g(|u|) \leq e^{-(1/2)T|u|} = g_o(|u|). 
$$

(3.7)

Now, (3.6) can be written in the form

$$
\lambda_1 = 1 - \min_\theta F(g, \theta) 
$$

where $g \geq g'$ implies $F(g, \theta) \geq F(g', \theta)$ for all $\theta$. It follows that for every $g$

$$
\min_\theta F(g_o, \theta) = F(g_o, \theta') \geq F(g, \theta') \geq \min_\theta F(g, \theta). 
$$

Hence,
\[ \lambda_1 \geq 1 - \min_{\theta} F(g_0, \theta) \]

and \( \lambda_1 \) is minimized by \( g_0 \). Q.E.D.

4. CONCLUSION

In this note we have established two results: (a) a general form of acceptance probability for constructing Gibbs fields, and (b) an optimality property for a particular choice of the acceptance probability, viz., that of the heat-bath model.

The results of this note can be generalized to continuous time Markov chains where (2.5) would apply to the acceptance rate, and under a boundedness condition on the rate (3.2) would yield an optimal acceptance rate.

References


