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# A GLOBAL SIMULATING ANNEALING METHOD *

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The Simulated Annealing method (SA)[1] aims to solve the problem of finding the value of a $N$–dimensional vector $\mathbf{x} \equiv (x_1, x_2, ..., x_N)$, such that the real function $E(\mathbf{x})$ takes its absolute minimum value. SA is inspired on an analogy with Statistical Physics: consider a fictitious physical system whose phase space is the set of variables $(x_1, \ldots, x_N)$ and whose energy is $E(\mathbf{x})$. If we heat the system to very high temperature $T$ and then *slowly* cool it down to the absolute zero (a process known as annealing), the system will reach the ground state, i.e. the state of minimum energy. The cooling rate needs to be slow enough in order to avoid getting trapped in some metastable state. According to Statistical Mechanics, the probability of a state with energy $E(\mathbf{x})$ at temperature $T$ is given by the Gibbs factor:

$$P(\mathbf{x}) \sim \exp(-E(\mathbf{x})/T). \tag{1}$$

For the implementation of the SA method, one must provide a manner of generating representative configurations at temperature $T$, and also a way of lowering the temperature with annealing step, $T(k)$. We have introduced[2] a SA method which uses global actualizations for the proposal of representative configurations via the Hybrid Monte Carlo algorithm (HMC)[3] in their generalized version[4]. We show that the method allows a more effective searching scheme and a faster annealing schedule, so improving upon the performance of other SA methods, mainly when the number of variables is large. In the generalized HMC method, the proposal change $\mathbf{x} \to \mathbf{x}'$ is generated by using a density probability function $g(\mathbf{x}'|\mathbf{x})$ in the following way: first, a set of initial values for the momenta $\mathbf{p}$ are generated by using the Gaussian distribution $\exp[-\mathbf{p}^2/2T]$; next, one introduces the mapping induced by $n$ iterations of the following basic step:

$$\begin{aligned} x_i' &= x_i + \delta t \sum_{j=1}^{N} A_{ij} p_j + \frac{\delta t^2}{2} \sum_{j,k=1}^{N} A_{ik} A_{jk} F_j(\mathbf{x}), \\ p_i' &= p_i + \frac{\delta t}{2} \sum_{j=1}^{N} A_{ji} [F_j(\mathbf{x}) + F_j(\mathbf{x}')], \qquad\qquad i = 1, \ldots, N, \end{aligned} \tag{2}$$

where $F_i(\mathbf{x}) = -\partial E(\mathbf{x})/\partial x_i$ is the "force" acting on the variable $x_i$, and $A_{ij}$ is an arbitrary matrix. This mapping is motivated by the numerical integration of the following equations of motion based on a Hamiltonian function $\mathcal{H}(\mathbf{x}, \mathbf{p}) = E(\mathbf{x}) + \mathbf{p}^2/2$:

$$\dot{x}_i = \sum_j A_{ij} p_j, \qquad \dot{p}_i = \sum_j A_{ji} F_j. \tag{3}$$

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which conserve energy, $\dot{\mathcal{H}} = 0$, and reduce to Hamilton's equations for $A_{ij} = \delta_{ij}$. As said earlier, the matrix $A_{ij}$ is arbitrary and, for instance, the choice $A_{ij} = A_i\delta_{ij}$ is equivalent to using an effective integration time step $\delta t_i = \mathcal{A}_i \delta t$ which is different for each variable:

$$x'_i = x_i + \delta t_i p_i + \frac{\delta t_i^2}{2} F_i(\mathbf{x}), \tag{4}$$
$$p'_i = p_i + \frac{\delta t_i}{2}[F_i(\mathbf{x}) + F_i(\mathbf{x}')], \qquad i = 1, \dots, N$$

Finally, the value $\mathbf{x}'$ should be accepted with the following probability:

$$h(\mathbf{x}'|\mathbf{x}) = \min\left(1, \exp\left[-\left(\mathcal{H}(\mathbf{x}', \mathbf{p}') - \mathcal{H}(\mathbf{x}, \mathbf{p})\right)/T\right]\right). \tag{5}$$

It can be shown that the above procedure satisfies the detailed balance condition, which is sufficient to ensure that the Gibbs distribution is being properly sampled.

The main advantage is that, by using this Hamiltonian based dynamics for the proposal of the new configuration, we use a global scheme for the actualizations. So, the global updates greatly increase the efficiency of the simulated annealing. In particular we are able to use quite generally an exponential annealing schedule: $T(k) = T_0 e^{-ck}$. Furthermore, since the acceptance decision in HMC is taken after all the $N$ variables have been updated, the number of energy function evaluations is greatly reduced.

In order to make a comparison with some representative SA algorithms proposed in the literature with ours, we have used a set of test functions which share the common feature of having many local minima close to the absolute one and we have compared our method with the Fast Simulated Annealing (FSA)[5], Very Fast Simulated Reannealing (VFSR)[6] and the Downhill Simplex with annealing (DSA)[7], which are considered to be amongst the best SA methods available. We have found that, in a large number of occasions, HSA requires orders of magnitude less evaluations of the function than the other methods in order to achieve a given accuracy in the minimum value of the function and can, therefore, yield a better solution in less computer time. This conclusion remains despite the fact that HSA requires some extra work when computing the evolution equations since it needs to compute also the forces $F_i$ acting on the different variables. These results show that the use of a global updating (Hybrid Monte Carlo) algorithm can indeed improve the performance of simulated annealing methods by allowing an effective searching scheme and fast annealing schedules. It is conceivable also that one could also use efficiently some of the acceleration schemes (Fourier, wavelet, etc.) which are easily implemented by simply choosing an appropriate expression for the matrix $A_{ij}$, in order to improve even further upon the convergence of the simulated annealing techniques.

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