Simulated Annealing in Optimization

Kuei-Yuan Chan, chanky@ntu.edu.tw
Professor of Mechanical Engineering,
National Taiwan University.

A robust method for seeking a global minimum must adopt a strategy where a higher value of a function is acceptable under some conditions. Simulated annealing provides such a strategy. Annealing is a process where stresses are relived from a previously hardened body. Parts with residual stresses are brittle and are prone to early failure. If a metal is heated to a high level of temperature, the atoms are in a constant state of motion. Controlled slow cooling allows the atoms to adjust to a stable equilibrium state of least energy. The probability $P(\Delta E)$ of change in energy ΔE is given by Boltzmann's probability distribution function given by

$$P(\Delta E) = e^{-\frac{\Delta E}{kT}} \tag{1}$$

where T is the temperature of the body and k is the Boltzmann's constant.

Metropolis observed that the energy can sometimes be increased in the annealing process even as the net change decreases. The optimization algorithm uses this concept is called the Metropolis algorithm. We start the algorithm at an initial temperature state, T, which is set at a high level. Boltzmann's constant can be set at 1. The change in objective function Δf is acceptable whenever it represents a decrease. When it is an increase, we accept it with a probability $P(\Delta E) = e^{-\Delta f/T}$. This is accomplished by generating a random number r between zero and one. The new value is acceptable if $r \leq P$.

Simulated-Annealing $(f, \mathbf{x}_0, N, t_0)$

$\triangleright t_0 \in \mathbf{R}$ is an initial temperature
$\mathbf{x} \leftarrow \mathbf{x}_0$
$t \leftarrow t_0$
while termination-condition()=FALSE **do**
  while repeating-condition()=FALSE **do**
    select $\mathbf{y} \in N(\mathbf{x})$
    if $f(\mathbf{y}) < f(\mathbf{x})$ **then**
      $\mathbf{x} \leftarrow \mathbf{y}$
      $\triangleright$ generate random number in $(0, 1]$
    else
      $r \leftarrow$ random(0,1)
      if $r \leq \exp\left(-\frac{f(\mathbf{y})-f(\mathbf{x})}{t}\right)$ **then**
        $\mathbf{x} \leftarrow \mathbf{y}$
      end if

end if

$t \to \mathrm{cool}(t)$ ▷ "cooling"

end while

end while

return $\mathbf{x}$