Adjusting the inverse temperature of the Boltzmann distribution

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1 Introduction

The Boltzmann distribution is a probability distribution having a parameter which controls the entropy. The parameter is called the inverse temperature. This report shows a method to adjust the inverse temperature so that the Boltzmann distribution has the given entropy. This method is firstly used for statistical evolutionary algorithms in [1].

2 Preliminary

2.1 The Boltzmann distribution

The Boltzmann distribution is defined by

$$q(x) = \frac{e^{-f(x)\beta}}{Z} \tag{1}$$

$$Z = \int e^{-f(x)\beta} dx, \tag{2}$$

where $f(x)$, β and Z are the energy function, the inverse temperature and the normalizing constant, respectively. The domain of β is $0 \leq \beta \leq \infty$. The normalizing constant is called the partition function since the normalizing constant is a function of β. If x is a element of a discrete set, the Boltzmann distribution is defined by using $\sum$ instead of $\int$.

2.2 The entropy of the Boltzmann distribution

The entropy of a probability distribution $p(x)$ is defined by

$$H = -\int p(x) \log p(x) dx. \tag{3}$$

Substituting (1) into (3), the entropy of the Boltzmann distribution is given by

$$H = \bar{f}\beta + \log Z, \tag{4}$$

where $\bar{f}$ is the average energy, defined by

$$\bar{f} = \int f(x) q(x) dx. \tag{5}$$

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3 The problem and its solution

The problem hilighted in this report is to find the inverse temperature so that the Boltzmann distribution has the given entropy, and we propose an approximation method.

The derivative of the entropy of the Boltzmann distribution with respect to the inverse temperature is given by

$$\frac{\partial H}{\partial \beta} = -\sigma^2 \beta, \tag{6}$$

where σ^2 is the variance of the energy, defined by

$$\sigma^2 = \int (f(x) - \bar{f})^2 q(x) dx. \tag{7}$$

The appendix would be helpful for deriving the derivative.

Let the entropy for the inverse temerature β denoted by $H(\beta)$ and the given entropy by $H(\beta^*)$. For any inverse temperature β_0 and β^*, the following equation holds:

$$H(\beta^*) = \int_{\beta_0}^{\beta^*} \frac{\partial H}{\partial \beta} d\beta + H(\beta_0). \tag{8}$$

However, the integration in (8) cannot be solved because the variance of the energy is a function of β.

Overcoming this difficulty, we assume that the variance of the energy is the constant value σ_0^2, which is the variance of the energh with $\beta = \beta_0$. In other words, it is supposed that the variance is not significantly changed by changing the inverse temperature. Then, we obtain

$$H(\beta^*) - H(\beta_0) = \int_{\beta_0}^{\beta^*} \frac{\partial H}{\partial \beta} d\beta \tag{9}$$

$$\simeq -\sigma_0^2 \int_{\beta_0}^{\beta^*} \beta \, d\beta \tag{10}$$

and thus

$$\beta^* = \sqrt{\beta_0^2 - \frac{2(H(\beta^*) - H(\beta_0))}{\sigma_0^2}} \qquad (\beta_0 < \beta^*) \tag{11}$$

where $\sigma(\beta)^2$ is the variance of the energy of the boltzmann distribution with the inverse temerature β.

References

[1] Takayuki Higo, "Research on the Importance Sampling Method for Evolutionary Algorithms Based on Probability Models", Doctor Thesis, Tokyo Institute of Technology, 2008.

A The Derivatives of $\log Z$

This section just provides simple calculations.

$$Z = \int e^{-f(x)\beta} dx \tag{12}$$

$$Z' = \int -f(x)e^{-f(x)\beta} dx \tag{13}$$

$$Z'' = \int -f^2(x)e^{-f(x)\beta} dx \tag{14}$$

$$\frac{\partial \log Z}{\partial \beta} = \frac{Z'}{Z} = -\bar{f} \tag{15}$$

$$\frac{\partial^2 \log Z}{\partial \beta^2} = \frac{z''z - (z')^2}{z^2} = \sigma^2 \tag{16}$$