Advanced Machine Learning Assignment: 3

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October 2024

The entropy of a system whose states are $\boldsymbol{x}$, at temperature $T = 1/\beta$ is

$$S = \sum p(\boldsymbol{x})[\ln \frac{1}{p(\boldsymbol{x})}]$$

where

$$p(\boldsymbol{x}) = \frac{1}{Z(\beta)} \exp[-\beta E(\boldsymbol{x})]$$

a

Show that

$$S = \ln Z(\beta) + \beta \bar{E}(\beta)$$

We start by filling in $p(\boldsymbol{x})$ into the formula for the entropy.

$$\sum p(\boldsymbol{x}) \left[\ln \left(\frac{1}{Z(\beta)} \exp[-\beta E(\boldsymbol{x})] \right)^{-1} \right]$$

We then work it out and simplify the terms:

$$= \sum p(\boldsymbol{x}) \left[- \ln \left(\frac{1}{Z(\beta)} \exp[-\beta E(\boldsymbol{x})] \right) \right]$$

$$= \sum p(\boldsymbol{x}) \left[- \ln \exp[-\beta E(\boldsymbol{x})] + \ln Z(\beta) \right]$$

$$= \sum p(\boldsymbol{x}) \left[\beta E(\boldsymbol{x}) + \ln Z(\beta) \right]$$

$$= \sum p(\boldsymbol{x}) \left[\beta E(\boldsymbol{x}) \right] + \sum p(\boldsymbol{x}) \left[\ln Z(\beta) \right]$$

$$= [\ln Z(\beta)] \sum p(\boldsymbol{x}) + \sum \frac{1}{Z(\beta)} \exp[-\beta E(\boldsymbol{x})] \left[\beta E(\boldsymbol{x}) \right]$$

$$= [\ln Z(\beta)] \sum p(\boldsymbol{x}) + \frac{\beta}{Z(\beta)} \sum \exp[-\beta E(\boldsymbol{x})] \left[E(\boldsymbol{x}) \right]$$

The function for $\bar{E}$ as specified in (31.6) of the book:

$$\bar{E} = \frac{1}{Z}\sum_{\boldsymbol{x}} \exp(-\beta E(\boldsymbol{x}))$$

This means the function comes out to:

$$= [\ln Z(\beta)] \sum p(\boldsymbol{x}) + \beta \bar{E}(\beta)$$

The sum over p adds up to 1, this means the final function is:

$$S = \ln Z(\beta) + \beta \bar{E}(\beta)$$

This is the function we have to show, so it is proven.

b

Show that

$$S = -\frac{\delta F}{\delta T}$$

, where the free energy $F = -kT \ln Z$ and $kT = 1/\beta$
In this case of F we set $k = 1$. This means the function F comes out to: $F = -T \ln Z$ and $T = \frac{1}{\beta}$
Then we take the derivative with the chain rule as Z includes T.

$$\frac{\delta F}{\delta T} = -\ln Z - T\frac{\delta \ln Z}{\delta T}$$

Expand the 2nd part of the derivative to include the derivative for beta

$$= -\ln Z - T\frac{\delta \ln Z}{\delta \beta}\frac{\delta \beta}{\delta T}$$

Replace T by $1/\beta$ and take the derivative. This comes out to $-\beta^2$
Substituting in the original formula gives:

$$= -\ln Z - \frac{1}{\beta}\left(\frac{\delta \ln Z}{\delta \beta}(-\beta^2)\right)$$

For $\frac{\delta \ln Z}{\delta \beta}$ fill in $-\bar{E}$ as described in (31.8) in the book. This gives:

$$= -\ln Z - \frac{1}{\beta}(-\beta^2)(-\bar{E})$$

$$= -\ln Z + (\beta)(-\bar{E})$$

This comes out to

$$-(\ln Z + \beta \bar{E})$$

which is indeed the negative of S. It is thus shown that this is the case.