



## Supplementary Material - Boosted Negative Sampling by Quadratically Constrained Entropy Maximization

Taygun Kekeç<sup>a</sup>, David Mimno<sup>b</sup>, David M. J. Tax<sup>a</sup>

<sup>a</sup>Pattern Recognition and Bioinformatics Laboratory  
Delft University of Technology  
Mekelweg 4 2628CD, Delft, The Netherlands

<sup>b</sup>Information Sciences Department, Cornell University  
Ithaca, NY 14853, New York

### ABSTRACT

This is the supplementary material for the paper titled "Boosted Negative Sampling by Quadratically Constrained Entropy Maximization".

© 2019 Elsevier Ltd. All rights reserved.

### Appendix A. Negative Sampling Objective

The negative sampling objective is given as follows:

$$J(\theta) = \mathbb{E}_{p_d} [\ln \sigma(\mathbf{x}; \theta)] + \mathbb{E}_{p_n^0} [\ln(1 - \sigma(\mathbf{y}; \theta))] \quad (\text{A.1})$$

Here,  $\sigma$  is the sigmoid function:

$$\sigma(\mathbf{u}; \theta) = \frac{1}{1 + \exp[-G(\mathbf{u}; \theta)]}$$

where  $G$  is the difference between the log likelihood of the sample under the model and the negative sampling distribution:

$$G(\mathbf{u}; \theta) = \ln p_m^\theta(\mathbf{u}) - \ln p_n(\mathbf{u})$$

Substitution of  $\sigma$  and  $G$  functions gives us the following:

$$J_T(\theta) = E_{p_d} \left[ \ln \frac{p_m^\theta(\mathbf{x})}{p_m^\theta(\mathbf{x}) + p_n(\mathbf{x})} \right] + \mathbb{E}_{p_n^0} \left[ \ln \frac{p_n(\mathbf{y})}{p_m^\theta(\mathbf{y}) + p_n(\mathbf{y})} \right]$$

Using logarithmic properties and expectation additivity, we decompose this objective into:

$$J(\theta, p_n) = \mathbb{E}_{p_d} [\ln p_m^\theta(\mathbf{x})] - \mathbb{E}_{p_d} [\ln(p_m^\theta(\mathbf{x}) + p_n(\mathbf{x}))] \\ - \mathbb{E}_{p_n^0(y)} [\ln(p_m^\theta(\mathbf{y}) + p_n(\mathbf{y}))] + \mathbb{E}_{p_n^0(y)} [\ln p_n(\mathbf{y})]$$

where fourth term is constant in  $\theta$ .  $\square$

### Appendix B. Smoothing the distribution

Assume we have a probability mass function, with *ordered* entries:

$$p_1 \geq p_2 \geq \dots \geq p_n > 0 \quad (\text{B.1})$$

with  $\sum_{i=1}^n p_i = 1$ . We smooth PMF  $p$  slightly, by modifying two neighbouring probabilities with a small probability  $\Delta_i$ . This defines a new PMF  $\tilde{p}$ , with  $\tilde{p}_i = p_i - \Delta_i$ ,  $\tilde{p}_{i+1} = p_{i+1} + \Delta_i$ , and all other probabilities remain the same. The entropy change:  $H(\tilde{p}) - H(p)$  can be stated as:

$$= -(p_i - \Delta_i) \log(p_i - \Delta_i) - (p_{i+1} + \Delta_i) \log(p_{i+1} + \Delta_i) \\ + p_i \log p_i + p_{i+1} \log p_{i+1} \\ = -p_i(\log(p_i - \Delta_i) - \log p_i) - p_{i+1}(\log(p_{i+1} + \Delta_i) - \log p_{i+1}) \\ + \Delta_i \log(p_i - \Delta_i) - \Delta_i \log(p_{i+1} + \Delta_i) \\ = -p_i(\log(1 - \frac{\Delta_i}{p_i})) - p_{i+1}(\log(1 + \frac{\Delta_i}{p_{i+1}})) \\ + \Delta_i \log(p_i(1 - \frac{\Delta_i}{p_i})) - \Delta_i \log(p_{i+1}(1 + \frac{\Delta_i}{p_{i+1}}))$$

The logarithms are of the form  $\log(1 + x)$  for which the Taylor expansion around  $x = 0$  can be used:

$$\log(1 + x) = 0 + x + O(x^2) \quad (\text{B.2})$$

*e-mail:* taygunkekec@gmail.com (Taygun Kekeç),  
mimno@cornell.edu (David Mimno), D.M.J.Tax@tudelft.nl (David M. J. Tax)

Therefore, the substitution gives:

$$\begin{aligned}
H(\tilde{p}) - H(p) &= p_i \frac{\Delta_i}{p_i} - p_{i+1} \frac{\Delta_i}{p_{i+1}} \\
&\quad + \Delta_i \log p_i - \Delta_i \frac{\Delta_i}{p_i} - \Delta_i \log p_{i+1} - \Delta_i \frac{\Delta_i}{p_{i+1}} + O(\Delta_i^2) \\
&= +\Delta_i \log p_i - \Delta_i \log p_{i+1} + O(\Delta_i^2) \\
&= \Delta_i \log \frac{p_i}{p_{i+1}} + O(\Delta_i^2) > 0
\end{aligned}$$

The first two terms cancel, the fourth and the sixth are of order  $O(\Delta_i^2)$ , and only the third and fifth term remain. Because  $p_i > p_{i+1}$ , this difference between the entropies  $H(\tilde{p}) - H(p)$  is larger than 0.  $\square$

### Appendix C. Powering the distribution

Assuming we have a probability mass function, as defined in Equation (B.1). We define a power  $\lambda$ ,  $0 < \lambda < 1$ , and rescale the PMF:

$$\tilde{p}_i = \frac{p_i^\lambda}{\sum_j p_j^\lambda} \quad (\text{C.1})$$

This new distribution is more smooth when

$$\hat{\Delta}_i \leq \Delta_i \quad (\text{C.2})$$

where  $\Delta_i = p_i - p_{i+1}$  That would mean:

$$\frac{p_i^\lambda - p_{i+1}^\lambda}{\sum_j p_j^\lambda} \leq p_i - p_{i+1}$$

$$p_i^\lambda - p_{i+1}^\lambda \leq \left(\sum_j p_j^\lambda\right)(p_i - p_{i+1}) \quad (\text{C.3})$$

$$p_i^\lambda - p_{i+1}^\lambda \leq C(p_i - p_{i+1}) \quad (\text{C.4})$$

This is actually the definition of Lipschitz continuity (Mohri et al., 2012). Unfortunately, for  $f(x) = x^\lambda$  where  $x \in [0, 1]$  and  $0 < \lambda < 1$  function  $f$  is *not* Lipschitz continuous, because for very small values of  $x$  the derivative goes to infinity.

If we now assume that  $\gamma < p_i < 1$ , our purpose is to derive a lower bound  $\gamma$  for  $p_i$  such that (C.3) actually holds. First, we define the function  $f$ :

$$\begin{aligned}
f(x) &= x^\lambda \quad x \in (0, 1), \quad \gamma < \lambda < 1 \\
f'(x) &= \lambda x^{\lambda-1} \quad \text{is always positive} \\
f''(x) &= \lambda(\lambda-1)x^{\lambda-2} \quad \text{is always negative}
\end{aligned}$$

in other words: the derivative is always positive, but each derivative becomes smaller and smaller. Because we have that  $x > \gamma$ , and for  $h > 0$ :

$$f'(\gamma) > f'(x) = \lim_{h \downarrow} \frac{f(x+h) - f(x)}{(x+h) - x} > \frac{f(x+h) - f(x)}{(x+h) - x} \quad (\text{C.5})$$

Using  $f'(x) = \lambda x^{\lambda-1}$ , and rewriting gives:

$$f(x+h) - f(x) < \lambda \gamma^{\lambda-1} ((x+h) - x) \quad (\text{C.6})$$

Substitution of  $x+h = p_i$  and  $x = p_{i+1}$  and solving  $\gamma$  reads:

$$p_i^\lambda - p_{i+1}^\lambda < \lambda \gamma^{\lambda-1} (p_i - p_{i+1}) \quad (\text{C.7})$$

Now we can identify  $\gamma$  using Equation (C.3):

$$\lambda \gamma^{\lambda-1} = \sum_j p_j^\lambda \quad (\text{C.8})$$

$$\gamma = \left( \frac{1}{\lambda} \sum_j p_j^\lambda \right)^{1/(\lambda-1)} \quad (\text{C.9})$$

(B.3) Now,  $\gamma$  gamma is lower bounded as such, powering the distribution acts as a smoother.  $\square$

### References

Mohri, M., Rostamizadeh, A., Talwalkar, A., 2012. Foundations of Machine Learning. The MIT Press.