Softmax

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My opinion on how and why softmax materializes. Consider the transformation

$$\mathbf{p} = \underset{\mathbf{w} \in \mathbf{S}}{\operatorname{argmin}} \langle \mathbf{w}, \mathbf{x} \rangle \tag{1}$$

where $\mathbf{x} \in \mathbf{R}^{\mathbf{d}}$, $\mathbf{w} \in \mathbf{S} \subset [0,1]^d$ such that $\mathbf{S} = \left\{ \mathbf{w} \mid \sum_{i=1}^d \mathbf{w}_i = 1 \right\}$, $\mathbf{p} \in [0,1]^d$ and $\sum_{i=1}^d \mathbf{p}_i = 1$. $\hat{\mathbf{p}}$ with entropy regularizer

$$\hat{\mathbf{p}} = \underset{\mathbf{w} \in \mathbf{S}}{\operatorname{argmin}} \langle \mathbf{w}, \mathbf{x} \rangle + \sum_{i=1}^{d} \mathbf{w}_{i} \log (\mathbf{w}_{i})$$
(2)

Since $\mathbf{w} \in \mathbf{S}$, add a Lagrange multiplier $\lambda (\langle \mathbf{w}, \mathbf{1} \rangle - 1)$ to the objective function.

$$\hat{\mathbf{p}} = \underset{\mathbf{w} \in \mathbf{S}}{\operatorname{argmin}} \langle \mathbf{w}, \mathbf{x} \rangle + \sum_{i=1}^{d} \mathbf{w}_{i} \log (\mathbf{w}_{i}) + \lambda (\langle \mathbf{w}, \mathbf{1} \rangle - 1)$$
(3)

$$= \underset{\mathbf{w} \in \mathbf{S}}{\operatorname{argmin}} \sum_{i=1}^{d} \mathbf{w}_{i} \mathbf{x}_{i} + \sum_{i=1}^{d} \mathbf{w}_{i} \log (\mathbf{w}_{i}) + \lambda \left(\sum_{i=1}^{d} \mathbf{w}_{i} - 1 \right)$$
(4)

(5)

Differentiate the objective function with respect to \mathbf{w}_i and equate to 0

$$\mathbf{x}_i + 1 + \log\left(\mathbf{w}_i\right) + \lambda = 0 \tag{6}$$

$$\mathbf{w}_{i}^{\star} = \exp\left(-\mathbf{x}_{i}\right) \exp\left(-1 - \lambda\right) \tag{7}$$

$$= \frac{\exp\left(-\mathbf{x}_i\right)}{\exp\left(1+\lambda\right)} \tag{8}$$

Set λ such that $\sum_{i}^{d} \mathbf{w}_{i}^{\star} = 1$

$$\mathbf{w}_{i}^{\star} = \frac{\exp(-\mathbf{x}_{i})}{\sum_{i=1}^{d} \exp(-\mathbf{x}_{i})}$$

$$\hat{\mathbf{p}} = \mathbf{w}^{\star}$$
(9)

$$\hat{\mathbf{p}} = \mathbf{w}^* \tag{10}$$

Reference

Luca Trevison. The "Follow-the-Regularized-Leader" algorithm. Topics in computer science and optimization (Fall 2019).