What Is the Softmax Function?

Nicholas J. Higham*

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The softmax function takes as input a real n-vector x and returns the vector g with elements given by

$$g_j(x) = \frac{e^{x_j}}{\sum_{i=1}^n e^{x_i}}, \quad j = 1:n.$$
 (*)

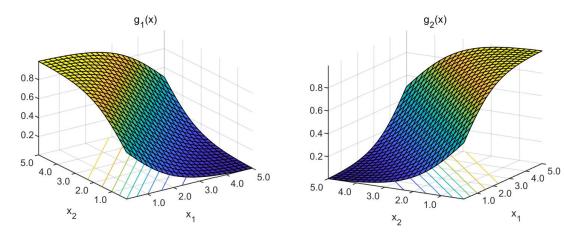
It arises in machine learning, game theory, and statistics. Since $e^{x_j} \ge 0$ and $\sum_{j=1}^n g_j = 1$, the softmax function is often used to convert a vector x into a vector of probabilities, with the more positive entries giving the larger probabilities.

The softmax function is the gradient of the log-sum-exp function

$$lse(x) = \log \sum_{i=1}^{n} e^{x_i},$$

where log is the natural logarithm, that is, $g_j(x) = (\partial/\partial x_j) \operatorname{lse}(x)$.

The following plots show the two components of softmax for n = 2. Note that they are constant on lines $x_1 - x_2 = \text{constant}$, as shown by the contours.



Here are some examples:

9.0031e-02

^{*}Department of Mathematics, University of Manchester, Manchester, M13 9PL, UK (nick.higham@manchester.ac.uk).

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2.4473e-01
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6.6524e-01

>> softmax([-1 0 10])

ans =

- 1.6701e-05
- 4.5397e-05
- 9.9994e-01

Note how softmax increases the relative weighting of the larger components over the smaller ones. The MATLAB function softmax used here is available at https://github.com/higham/logsumexp-softmax.

A concise alternative formula, which removes the denominator of (*) by rewriting it as the exponential of lse(x) and moving it into the numerator, is

$$g_j = \exp(x_j - \operatorname{lse}(x)). \tag{#}$$

Straightforward evaluation of softmax from either (*) or (#) is not recommended, because of the possibility of overflow. Overflow can be avoided in (*) by shifting the components of x, just as for the log-sum-exp function, to obtain

$$g_j(x) = \frac{e^{x_j - \max(x)}}{\sum_{i=1}^n e^{x_i - \max(x)}}, \quad j = 1: n.$$
 (†)

where $\max(x) = \max_i x_i$. It can be shown that computing softmax via this formula is numerically reliable. The shifted version of (#) tends to be less accurate, so (\dagger) is preferred.

References

This is a minimal set of references, which contain further useful references within.

- Pierre Blanchard, Desmond J. Higham, and Nicholas J. Higham, Accurately Computing the Log-Sum-Exp and Softmax Functions, IMA J. Numer. Anal., Advance access, 2020.
- Bolin Gao and Lacra Pavel, On the Properties of the Softmax Function with Application in Game Theory and Reinforcement Learning, ArXiv:1209.5145, 2018.
- Ian Goodfellow, Yoshua Bengio, and Aaron Courville, Deep Learning, MIT Press, 2016.

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