

CAN A CONVEX PARTITION CAUSED BY A CPWL NEURAL NETWORK BE USED FOR DENSITY ESTIMATION?

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The increasing popularity of deep learning methods has led to a growing interest in understanding the theoretical properties of neural network. The use of information theory, as proposed by Tishby & Zaslavsky (2015); Shwartz-Ziv & Tishby (2017), provides a promising framework for studying the behaviour of these models. However, calculation of information theoretic (IT) quantities rely on estimating high-dimensional probability densities, which is challenging. Geiger (2022) show that the numerical results of different IT-measures vary depending on which estimator is used. In an attempt to combat this, we want to use the convex partitioning properties of Continuous Piecewise Linear (CPWL) neural network, such as ReLU networks, in order to create “natural bins” of the models input and latent spaces.

A ReLU network will partition its input space into convex regions (Serra et al., 2018; Hanin & Rolnick, 2019a). The number of regions is upper bounded by 2^H where H is the total number of hidden units in the network. However, only a few of these are considered feasible regions Hanin & Rolnick (2019b). Finding these regions for the whole network is previously explored by Liu et al. (2023); Sattelberg et al. (2023); Humayun et al. (2024). However, all of these approaches are limited to specific cases, or weak numerical implementations. Our goal is to create a more general and scalable algorithm for finding the feasible regions of ReLU network, both for the whole network and for each layer. The ultimate goal is to use these regions as bins when performing density estimation for IT-measures. See Figure 1 for a preliminary example of how a random layer with three neurons partitions its two-dimensional input space.

If successful, this could provide a more principled way of estimating IT-measures for neural networks, free from arbitrary choices of binning or kernel sizes and other hyperparameters. In addition, we would be able to compute the mutual information between input and output, based on how the network partitions the input space. We hypothesize that mutual information should increase as the network learns how to partition input space in a feasible way. Furthermore, we should be able to spot bottlenecks in the network, by looking at how the number of regions changes from layer to layer throughout training.

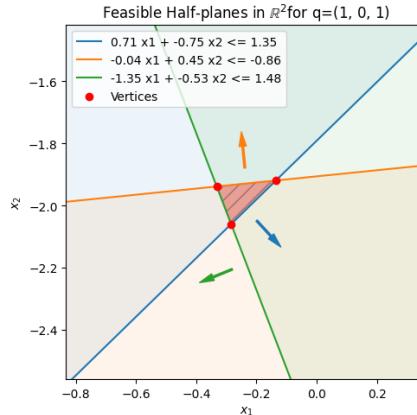


Figure 1: Preliminary example. Random layer, $\mathbb{R}^2 \rightarrow \mathbb{R}^3$, divides its input space into 7 convex regions. The activation vector $q = [1, 0, 1]$ (indicating which neuron is active) corresponds to the red region. Each activation pattern corresponds to a convex region in input space, of which there can be at most 2^H . Only a subset are feasible. For more complex layers and networks, the idea is that these regions can be used as “natural bins” when estimating information theoretic quantities.

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