A Probabilistic Interpretation of Transformers
International Conference on Machine Learning (ICML 2021)

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Abstract

This document provides a basic paper template and submission guidelines. Abstracts must be a single paragraph, ideally between 4–6 sentences long. Gross violations will trigger corrections at the camera-ready phase.

1. Introduction

Transformers have reached state of the art results in language models, significantly outperforming LSTMs. One conceptual explanation for their increased performance is the ability of attention to utilize long range dependencies, whereas Recurrent Neural Networks were limited by having to encode past information within a fixed size hidden state. What this explanation does not explain is how certain architectural choices of transformers, specifically exponential dot product attention, also somewhat ambiguously referred to as softmax attention, outperforms alternatives.

Exponential dot product attention has been seen before in contrastive learning, though often with normalized embeddings before softmax is applied. In language models, the softmax probability was used in Word2Vec and later word embedding work and for memory networks it was used in Neural Turing Machines. Contrastive loss originated as Noisy Contrastive Estimation and continues to be used in seminal papers such as SimCLR, which achieved state of the art results, as have many variants based off SimCLR.

The successes of transformers has been verified empirically, but far research has focused on a theoretical explanation of transformers perform so well. We offer a probabilistic explanation, based off of distributions of the exponential family, for attention and contrastive probabilities. Expressing attention as an exponential family allows us to utilize related theory in statistics, machine learn- ing, and statistical mechanics, offering insightful interpretations in to the transformer architecture.

We also explicitly state the limitations of our theory, noting that the modern Hopfield network interpretation shares many of these limitations. Moreover, for some of these limitations, we speculate connections between other areas of research which may reconcile the theoretical inconsistencies, motivating directions for future research.

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2. Related Work

3. Exponential Dot Product Attention

Word2vec used a skip-gram model to predict neighboring words using a conditional distribution defined by a normalized exponential dot product multinoulli function (Mikolov et al., 2013)

Attention was proposed through normalized exponential alignment functions, often referred to as softmax attention in literature, for Neural Machine Translation (Graves, 2013; Bahdanau et al., 2014), and later work parallelizing computation on sequential data introduced normalized exponential dot product similarity (Parikh et al., 2016) (A Decomposable Attention Model for Natural Language Inference). Neural Turing Machines gated memory updates using normalized exponential cosine similarity, in what is referred to as soft attention (Graves et al., 2014).

Other transformer precursors parallelized attention updates over the entire sequence into a layer and switched to convolution-based attention weights (Kaiser & Sutskever, 2016; Kaiser & Bengio, 2016). The transformer architecture incorporated exponential dot product attention scaled by dimensionality (Vaswani et al., 2017).

3.1. Contrastive Learning and Metric learning

Noise-Contrastive Estimation creates a mixture distribution between real data and noisy data to convert an unsupervised learning problem into a semi-supervised learning problem, modeling the distribution of the class conditioned on the data sample as a bernoulli distribution, and using the ratio of the model data distribution and noise distribution to define the logits (Gutmann & Hyvärinen, 2010).

In metric learning, Multidimensional scaling calculates pairwise distances between projected points (Cox & Cox, 2000), and for Euclidean distances it is equivalent to PCA (Bishop, 2007) Bishop, which uses dot products in calculating a covariance matrix. Neighborhood Components Analysis learns a low dimensional linear embedding matrix and models a probability of a neighbor by comparing the exponential negative distance to a neighbor to the sum of the exponential negative distances to non-neighbors (Goldberger et al., 2004)

Due to slow convergence of Bernoulli contrastive loss and triplet loss, Sohn proposed an exponential dot product probability over multiple examples (Sohn, 2016), which is mathematically consistent with NCE for multiple distributions. The papers roots in metric learning motivated the dot product form, with a direct influence from Neighborhood Component Analysis.

More recent contrastive learning research adopted a contrastive loss based off of exponential dot product probabilities, including papers that achieve state of the art semi-supervised learning (**?**).

3.2. Shortcut connections and dynamical systems

Long Short-Term Memory (LSTM) combined a shortcut connection to deal with the vanishing and exploding gradient problem along with gating functions to incorporate and forget information (Hochreiter & Schmidhuber, 1997). Residual connections similarly formulated the hidden layer as an update to an identity mapping, though without a gating mechanism (He et al., 2015). Recurrent Neural Networks have been interpreted as a discrete time approximation to a continuous dynamical system (Jaeger, 2001), where gating acts as a warping of time (Tallec & Ollivier, 2018). Residual connections have been interpreted as a discretized update to a differential equation (Weinan, 2017; Lu et al., 2020).

Interpreting residual networks as discretized differential equations, researchers have posed alternative methods for performing forward updates to converge to equilibrium points and backwards updates to the parameters from the equilibrium points (Chen et al., 2019; Bai et al., 2019). Further work has used monotone operator theory in convex analysis for solving for equilibrium points, interpreting layers as an operator (Winston & Kolter, 2021).

In a work most similar to ours, transformers have been interpreted as an update of modern hopfield networks and fixed points have been calculated with respect to a fixed set of patterns (Ramsauer et al., 2020). Our work similarly views the attention sublayer as an operator update over a class of discretized probability distribution, though with a changing set of patterns.

3.3. Log normalizer and free energy

Partition functions, or the normalizer function, in statistical physics defines a normalization factor of the Hamiltonian with respect to a parameter defining the temperature. The Boltzmann distribution can be derived through Lagrange multipliers as the distribution which maximizes entropy with a conservation of energy constraint. Jaynes adapted the Boltzmann distributions to maximum entropy distributions with multiple expected statistics constraints by converting the maximum entropy problem into the dual problem of optimizing the log normalizer (Jaynes, 1982), which is known in statistical mechanics as free energy.

Variational methods have been used to approximate log probabilities of observations in machine learning, borrowing from ideas in statistical mechanics. By viewing the joint as an unnormalized probability distribution, the log normalizer is known as the evidence lower-bound, and it has connections to Helmholtz Free Energy (Hinton et al., 1995; Koller & Friedman, 2009).

The sum of exponents loss of AdaBoost (Collins et al., 2000) has been interpreted as the dual form of generalized KL divergence. The log sum of exponents is well known in convex optimization to be the dual form to the maximum entropy objective for a discrete probability distribution (Boyd & Vandenberghe, 2004). Notably, in the modern Hopfield network interpretation of transformers as part of the energy function (Ramsauer et al., 2020).

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0.25 inches of space before the heading and 0.15 inches after the heading.

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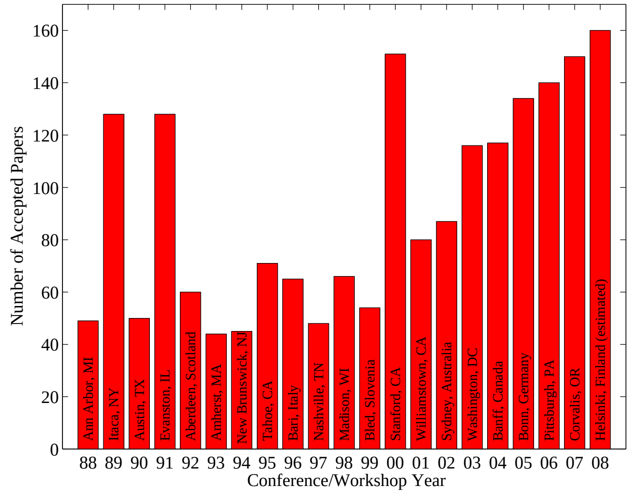

Figure 1. Historical locations and number of accepted papers for International Machine Learning Conferences (ICML 1993 – ICML 2008) and International Workshops on Machine Learning (ML 1988 – ML 1992). At the time this figure was produced, the number of accepted papers for ICML 2008 was unknown and instead estimated.

Algorithm 1 Bubble Sort

Input: data x_i, size m
repeat
  Initialize $noChange = true$.
  for $i = 1$ **to** $m - 1$ **do**
    if $x_i > x_{i+1}$ **then**
      Swap x_i and x_{i+1}
      $noChange = false$
    end if
  end for
until $noChange$ is $true$

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Table 1. Classification accuracies for naive Bayes and flexible Bayes on various data sets.

DATA SET	NAIVE	FLEXIBLE	BETTER?
BREAST	95.9± 0.2	96.7± 0.2	√
CLEVELAND	83.3± 0.6	80.0± 0.6	×
GLASS2	61.9± 1.4	83.8± 0.7	√
CREDIT	74.8± 0.5	78.3± 0.6	
HORSE	73.3± 0.9	69.7± 1.0	×
META	67.1± 0.6	76.5± 0.5	√
PIMA	75.1± 0.6	73.9± 0.5	
VEHICLE	44.9± 0.6	61.5± 0.4	√

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