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, sig- nificantly outperforming LSTMs. One conceptual explanation for their in- creased performance is the ability of attention to utilize long range dependencies, whereas Recurrent Neural Networks were limited by having to encode past infor- mation 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 learn- ing, 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 Ma- chines. Contrastive loss originated as Noisy Contrastive Estimation and contin- ues 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.

2. Related Work

2.1. Contrastive Learning

2.2. 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.

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2.3. 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).

3. Electronic Submission

Submission to ICML 2021 will be entirely electronic, via a web site (not email). Information about the submission process and LaTeX templates are available on the conference web site at:

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- Submissions must be in PDF.
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- **Do not include author information or acknowledgements** in your initial submission.
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Paper Deadline: The deadline for paper submission that is advertised on the conference website is strict. If your full, anonymized, submission does not reach us on time, it will not be considered for publication.

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```

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The final versions of papers accepted for publication should follow the same format and naming convention as initial submissions, except that author information (names and affiliations) should be given. See Section 4.3.2 for formatting instructions.

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[1] Footnotes should be complete sentences.

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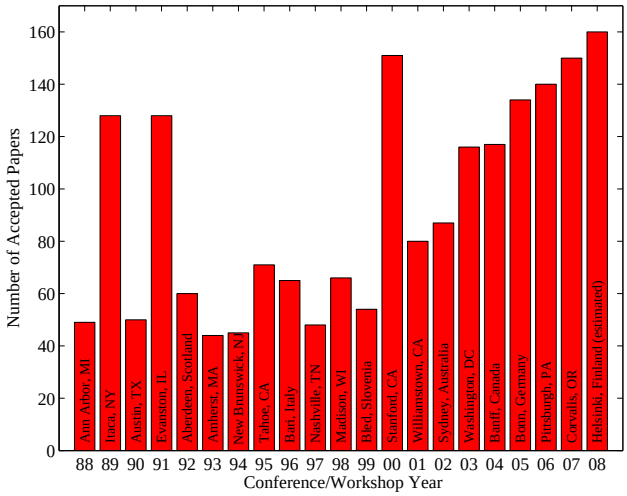

Figure 1. Historical locations and number of accepted papers for International Machine Learning Conferences (ICML 1993 – ICML 2008) and International Workshops on Machine Learning (ML 1988 – ML 1992). At the time this figure was produced, the number of accepted papers for ICML 2008 was unknown and instead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

4.7. Algorithms

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You may also want to include tables that summarize material. Like figures, these should be centered, legible, and numbered consecutively. However, place the title *above* the table with at least 0.1 inches of space before the title and the same after it, as in Table 1. The table title should be set in 9 point type and centered unless it runs two or more lines, in which case it should be flush left.

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	√

Tables contain textual material, whereas figures contain graphical material. Specify the contents of each row and column in the table's topmost row. Again, you may float tables to a column's top or bottom, and set wide tables across both columns. Place two-column tables at the top or bottom of the page.

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