RETENTION BASED AUTOREGRESSIVE MODELS FOR MODELLING NEURAL DYNAMICS

BY

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ABSTRACT

Retention based autoregressive models for modelling neural dynamics

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In this work, we present Retention, a novel autoregressive model for generative modelling of sequences. Unlike Transformer based autoregressive models, retention scales linearly with respect to context size. We apply retention based models for modelling neural dynamics and achieve SOTA performance in neural modelling and behaviour decoding.

To Mom,
   who did something nice.

ACKNOWLEDGEMENTS

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PUBLICATIONS

This work has not been published yet.

CONTENTS

INTRODUCTION

Hard problems inspire the creation of novel algorithms. These novel algorithms then find application in various contexts, distant from the original application which it was designed for. Understanding the human brain, specifically its dynamics and the relationship between dynamics of the brain and behaviour is a hard problem. Unraveling the dynamics of the brain holds the key to understanding the neural mechanisms underlying these processes. Beyond modeling neural activity, elucidating how such activity correlates with an organism's behavior is crucial for developing Brain-Computer Interfaces, clinical treatments for conditions like epilepsy, depression, and other neurodegenerative diseases. In this thesis, we develop scalable methods for modelling neural dynamics and relationship between the dynamics of the brain and behaviour. Although methods in this thesis are developed specifically for neural data, we believe that our approach would find application in diverse sequence modelling tasks in language, finance and engineering.

Machine learning techniques have played a pivotal role in modeling brain dynamics, and modeling the correlation between neural dynamics and behavior of an animal. In [POC+18], Pandarinath et al. introduced LFADS, an RNN-based method to infer latent dynamics from neural data. More recently, transformer-based models [VSP+17, GZ22], have been applied to learn neural dynamics and behaviour model. In [YP21], Pandarinath et al applied transformer-based models to learn neural dynamics without an explicit dynamical model. While LFADS and NDT (Neural Data Transformers) were focused on learning neural dynamics from single trial recordings, Azabou et.al recently introduced POYO [AAG+23], a transformer-based model to learn neural dynamics from multi-session neural recordings.

Although transformer-based models have shown remarkable success in general language modelling tasks and more recently in learning population dynamics of neurons, they exhibit poor scaling properties especially when applied to neural spiking data. Furthermore, unlike text data, neural recording probes sample on the order of kHz, and hence are characterized by high temporal resolution. This unique temporal aspect of neural

spiking data presents a challenge for transformers, which are originally designed for sequential data but may struggle with the high-frequency nature of neural signals. The transformer's poor scaling properties become particularly evident when recording from a large number of neurons simultaneously, as the number of potential firing patterns exponentially increases with the number of neurons.

In this work, we introduce a new class of autoregressive models to overcome limitations imposed by the architecture of attention-based transformer models. Our model has an unbounded context length and hence can capture long-range dependencies in the time series dataset. Furthermore, the complexity of training and inference of the parametrized model is independent of the context length, and hence our approach is computationally more efficient when compared to transformer-based autoregressive models.

PROBLEM STATEMENT

Imagine we are recording data from D neurons distributed across different regions of the brain. Let $x(t_i) \in \mathbb{R}^D$ denote the observed neural activity at timestep t_i and let y_i denote the observed behaviour of the animal at timestep t_i. From the time series dataset $\mathcal{D} = \{(x_i, y_i, t_i)\}_{i=1}^N$ of neural recordings, our goal is to construct:

- A predictive model of underlying brain dynamics

- A probabilistic model to predict behaviour of the organism at time $t + 1$ given brain recordings until timestep t.

More formally, let's assume that the spiking activity is generated by an underlying non-stationary stochastic process defined by $p_t(x)$.

$$x(t) \sim p_t(x) \tag{2.1}$$

The probability of observing a sequence of neural recordings and behavior can be expressed as:

$$p(\{x_1, y_1\}, \{x_2, y_2\}, \{x_3, y_3\}, ..) = \lim_{N \to \infty} \prod_{i=1}^N p(\{x_i, y_i\} | \{x_1, y_1\}, \{x_2, y_2\}, ..\{x_{i-1}, y_{i-1}\})$$

$$\tag{2.2}$$

In the context of neural recordings, it is convenient to assume that the neural recording data and behavior can be modelled with separate probability distributions of the form:

$$\prod_{i=1}^N p_d(\{x_i\} | \{x_1\}, \{x_2\}, ..\{x_{i-1}\}) \tag{2.3}$$

$$\prod_{i=1}^N p_b(\{y_i\} | \{x_1\}, \{x_2\}, ..\{x_{i-1}\}) \tag{2.4}$$

Specifically, we assume that that the neural observed neural spiking data at timestep t_i is not dependent on the behavior variables in the preceding timesteps. Probability distributions of this nature have been extensively investigated in the field of language modeling. In conventional autoregressive frameworks, the approximation of conditional distributions often involves the utilization of parameterized models constrained by a finite

context limit [VSP$^+$17]. While autoregressive models of this kind have been extremely successful in generating plausible language [RNS$^+$18], they still struggle to capture long-range dependencies due to the finite context length limit[Hah20]. Furthermore, the complexity of training and inference of transformer-based models is $\mathcal{O}(N^2)$, where N is the context length of the transformer model.

METHODS

In this chapter, we describe the theory behind Retention based autoregressive models and methods for training retention based models.

3.1 MOTIVATION

To model conditional distributions defined in eq(2.4) exactly, we require a method that can process sequences of variable input length. In the realm of neural spiking data, which is frequently recorded at a sampling rate expressed in kHz, we require a method that can efficiently scale with the length of the sequence Furthermore, the patterns of neural activity increase exponentially with respect to the number of neurons, and hence the number of discrete tokens required to represent neural spike pattern at time step t can be prohibitively large. For instance, if we are recording spike signals from 100 neurons, in total there are 2^{100} possible firing patterns. Existing Transformer based models cannot be directly applied to model conditional distributions of these kind, without placing an assumption on the nature of probability distribution.

To address these challenges, we introduce "Retention", a mathematical operation to map a sequence of vectors $\{x_i\}_{i=1}^N$ to real valued vector ζ_i of same dimension. Retention is inspired from Score-life programming [Mur23], a novel method to solve sequential decision making problems. In Score-life programming [Mur23], Muraleedharan et.al applied the insight that the binary expansion of a real number can be used to represent a sequence of discrete variables. After constructing the mapping between a sequence of discrete variables and real numbers in a bounded interval, functions can be directly defined on the real numbers. By defining functions using this approach, we can model non-trivial relationships between elements of a sequence. In prior work [Mur23], has showed that such functions have unique properties, which can be exploited in developing efficient methods for solving determinsitic reinforcement learning problems. In our work, we extend this insight to vector valued variables, which are typically encountered in deep learning settings.

3.2 RETENTION

Mathematically, retention is defined as an exponentially weighted sum of a sequence of discrete vectors. If the vectors are drawn from a continuous space, then we perform thresholding operation to discretize the vectors. Specifically, given a sequence of vectors $\{x_i\}_{i=1}^N$, $x_i \in \mathbb{R}^d$, Retention variable $\zeta_k \in [0,1)^d$ as:

$$\zeta_k = \sum_{j=1}^{k} 2^{-(\log M)j} \sum_{i=0}^{M-1} \sigma(w_i \otimes x_{k-j+1} + b_i) \qquad (3.1)$$

Here, $w_i, b_i \in \mathbb{R}^d$ are trainable parameters for the thresholding operation defined in inner summation. Given a vector $x_i \in \mathbb{R}^d$ as input, the inner summation operation acts like a smoothened step function, essentially discretizing elements of the vector to discrete values in the set: $\{0, 1, 2, , , M-1\}$. The outer summation operation, with an exponentially decaying factor maps the sequence of discrete vectors to a continuous real valued vector ζ_k. If the input data is discrete, or binary as in the case of neural spike signals, then the thresholding operation can be omitted, and the retention variable can be defined as:

$$\zeta_i = \sum_{k=1}^{i-1} 2^{-k}(x_{i-k}) \qquad (3.2)$$

Given a sequence of discrete vectors $\{x_i\}_{i=1}^N$, retention variable ζ_i stores the discrete vectors in the binary expansion of ζ_i. If the vectors $\{x_i\}_{i=1}^N$ are continuous, then we perform a thresholding operation first to discretize the vectors and perform discounted sum of these discretized vectors.

Retention can also be defined for sequence of matrices $\{\mathbf{X}_i\}_{i=1}^N$ as:

$$\mathbf{1}_k = \sum_{j=1}^{k} 2^{-(\log M)j} \sum_{i=0}^{M-1} \sigma(\mathbf{W}_i \otimes \mathbf{X}_{k-j+1} + \mathbf{B}_i) \qquad (3.3)$$

Modelling Conditional Distributions with Retention Variables

Now, we approximate the conditional distribution defined in eq(3) with retention. Specifically, the product of conditional distributions can now be approximated as:

$$\prod_{i=1}^{N} p_d(\{x_i\}|\{x_1\}, \{x_2\}, ..\{x_{i-1}\}) \approx \prod_{i=1}^{N} p_d(\{x_i\}|\zeta_i) \qquad (3.4)$$

In this case, we

To learn the dynamics of the brain from neural recordings in an unsupervised manner, we maximize the following likelihood:

$$\mathcal{L}(X, \theta) = \sum_i log(p_d(\{x_i\}|\zeta_i; \theta)) \tag{3.5}$$

Here, $X = \{x_1, x_2, ...x_M\}$, the dataset of neural recordings.

Note that in this approach, the context window is not bounded, and the complexity of learning the parametrized model $p_d(\{x_i\}|\zeta_i; \theta)$ is independent of the length of the context window. While training the model, we apply eq(6) to recursively update ζ_i in an online fashion, instead of pre-computing and storing $\{\zeta_i\}_{i=1}^N$ separately.

To learn the correlation between neural dynamics and behavior, we follow a similar approach and approximate the conditional distribution defined in eq(4) with:

$$\prod_{i=1}^N p_b(\{y_i\}|\{x_1\}, \{x_2\}, ..\{x_{i-1}\}) \approx \prod_{i=1}^N p_b(\{y_i\}|\zeta_i) \tag{3.6}$$

We define the loss function associated with this approach as the negative log-likelihood of the observed behavioral outcomes given the estimated neural activity states. Formally, the loss function $\mathcal{L}$ is expressed as:

$$\mathcal{L}(X, Y, \phi) = -\sum_i \log p_b(\{y_i\}|\zeta_i; \phi)$$

3.3 TRAINING RETENTION BASED MODELS

In this section, we describe how retention based models are trained.

Online Computation of Retention Variable

Offline Computation of Retention Variable

3.4 ARCHITECTURE

Two Photon Dataset: U-Net

Fully connected networks

4

RESULTS

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4.1 A NEW SECTION

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4.3 SOME MATH

We can define scalar multiplication in $\mathbb{R}^n$ by

$$c[u_1, \ldots, u_n] = [cu_1, \ldots, cu_n]$$

You can now check that for $u, v \in \mathbb{R}^n$, we have

$$c(u + v) = cu + cv$$

5

CONCLUSION

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