# DIMENSIONALITY REDUCTION TECHNIQUES APPLIED TO NEURON FIRING DATA AIM TO INVESTIGATE AND QUANTIFY THE CORRELATION BETWEEN SPECIFIC HORMONES AND BEHAVIORS

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**THESIS**

Submitted in Partial Fulfillment of
the Requirements for
the Degree of

**Master of Science in Computer Science**

at the

**NEW YORK UNIVERSITY**
**TANDON SCHOOL OF ENGINEERING**

by

Aya Oshima

September 2024

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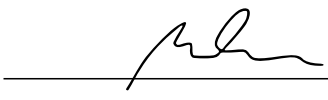

Department Chair Signature

Date September 8, 2024

# Approved by the Guidance Committee

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Date Aug 29,2024

**Advisor's Name:** Edward Wong

**Professional Rank:** Associate Professor

**School Affiliation:** NYU Tandon School of Engr

**Date:** Sept 2, 2024

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**School Affiliation:** NYU Tandon School of Engineering

**Date:** 8/30/2024

# Vita

Aya is an AI engineer and a Master of Science candidate in Computer Science at NYU Tandon School of Engineering, with a focus on Artificial Intelligence (AI) and Machine Learning (ML). Her academic and research pursuits centre on computational neuroscience, neurotechnology, and the integration of AI with business innovation. She is driven by a commitment to advancing our understanding of the human brain through AI, while simultaneously ensuring that technological advancements are aligned with ethical imperatives and the protection of fundamental human rights.

Aya is particularly interested in the convergence of AI, neuroscience, and cognitive science. Her work seeks to explore brain-machine interfaces (BMI) as a frontier for enhancing human capabilities and cognitive functions. She is dedicated to fostering interdisciplinary research that merges technical expertise with ethical frameworks, aiming to push the boundaries of what is possible in AI and neurotechnology in ways that are socially responsible and transformative.

Aya's research is focused on the following areas:

- **Brain-Machine Interfaces (BMI)**: Investigating innovative approaches for interfacing the human brain with machines to enhance cognitive abilities and develop novel human-augmentation technologies.
- **Neurotechnology**: Advancing non-invasive techniques for monitoring and modulating neural activity, contributing to both foundational neuroscience and its practical applications in technology.
- **AI and Business Innovation**: Examining how AI methodologies can be strategically deployed in business contexts to optimise decision-making processes, drive efficiency, and foster innovation.

# Acknowledgments

I would like to express my sincere gratitude to my advisor, Dr. Robert Froemke, for their continuous support, guidance, and invaluable feedback throughout this journey. I am also thankful to my committee members, Dr. Robert Froemke, Dr. Edward Wong, and Mo Satt, MS, for their insightful comments and encouragement.

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My heartfelt thanks to NYU Tandon for the overall opportunity to pursue this work and for supporting my academic journey.

I am also thankful to Dr. Robert Froemke's lab for their assistance, collaboration, and sharing of insightful data.

Lastly, I would like to acknowledge the funding agencies and institutions that supported this research.

## ABSTRACT

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**Dimensionality reduction techniques applied to neuron firing data aim to investigate and quantify the correlation between specific hormones and behaviors**

by

**Aya Oshima**

Advisor: **Dr. Robert Froemke**

Submitted in Partial Fulfillment of the Requirements for
Master of Science in Computer Science

September 2024

This thesis presents a comprehensive investigation into the neural mechanisms underlying maternal behavior learning, leveraging advanced computational methodologies to decode the complex patterns of neural activity. Through the application of Tensor Component Analysis (TCA), this research systematically dissects high-dimensional neural data, revealing the latent structures and dynamic processes that are critical for understanding how the brain encodes behavioral information.

The study is anchored in a series of rigorously controlled experiments that explore the differential impact of active versus passive engagement on neural dynamics within the paraventricular nucleus (PVN), a key region implicated in oxytocin-mediated behaviors. By contrasting direct physical interaction with screen-based observational learning paradigms, the research identifies significant enhancements in neural synchrony and circuit coherence associated with active participation. These findings indicate that active engagement in the learning process leads to a more robust and temporally precise neural representation of maternal behaviors, suggesting a critical role for sensory-motor integration in shaping effective neural encoding.

Beyond these empirical insights, this thesis introduces a methodological frame-

work that integrates TCA into the study of complex neural datasets, offering a novel approach for exploring the intricate relationships between neural structure and function. The application of TCA in this context not only advances our understanding of the specific neural circuits involved in maternal behavior but also demonstrates the utility of this technique in broader neuroscientific inquiries.

In addition to its immediate contributions, this work lays the foundation for future research into the neural basis of behavior, providing both theoretical insights and practical methodologies that can be extended to other domains. The findings underscore the importance of active learning in the effective encoding of behavioral information, offering new perspectives on how engagement shapes the brain's neural networks.

This research is positioned at the intersection of computational neuroscience and behavioral science, contributing to a deeper understanding of the neural dynamics that underpin complex behaviors. The methodologies and insights developed in this thesis are expected to inform and inspire further explorations into the brain's capacity for learning and adaptation.

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# Introduction

Understanding the neural mechanisms underlying maternal behavior is a critical area of research in neuroscience, with significant implications for both basic science and potential clinical applications. Maternal behavior, particularly in mammals, is a complex and highly adaptive process governed by intricate neural circuits and neurochemical systems. Among these, the role of the hypothalamic paraventricular nucleus (PVN) and the neuropeptide oxytocin has garnered considerable attention. Oxytocin, often dubbed the "love hormone," is crucial in regulating social behaviors, including bonding, trust, and caregiving. Despite extensive research, the precise neural dynamics that facilitate maternal behavior, especially in non-biological parenting (alloparenting), remain poorly understood.

This thesis aims to bridge this knowledge gap by exploring the neural mechanisms that govern the learning and expression of maternal behaviors in mice, focusing on the PVN and its modulation by oxytocin. The study is particularly concerned with how virgin mice, which lack inherent maternal instincts, learn maternal behaviors through social transmission, a process hypothesized to be heavily influenced by neural plasticity in response to social cues.

A significant challenge in neuroscience is the analysis of complex neural data, such as spike-trains, to uncover the underlying neural mechanisms driving behavior. Traditional methods often fall short in capturing the multidimensional and dynamic nature of neural activity, especially in tasks involving learning and social interaction. To address this, the thesis employs Tensor Component Analysis (TCA), a powerful computational tool that allows for the decomposition of high-dimensional neural data into interpretable components. By applying TCA to data collected from experiments involving active and passive engagement in maternal behavior learning, this research seeks to elucidate the distinct neural patterns associated with different levels of behavioral engagement.

**Research Objectives**

The primary objectives of this thesis are as follows:

1. **To model the global neural activity of the PVN**: By analyzing the neural activity recorded during different stages of maternal behavior learning, the study aims to model the PVN's role in facilitating these behaviors.

2. **To apply Tensor Component Analysis (TCA) to neural data**: The thesis seeks to leverage TCA to identify and differentiate neural patterns associated with varying levels of engagement in learning maternal behaviors. This includes

comparing active engagement, where mice actively seek out learning opportunities, to passive engagement, where learning is imposed without volition.

3. **To investigate the effective connectivity between neurons**: Using information-theoretic measures, the study will explore how the PVN neurons interact during different stages of learning, shedding light on the neural circuits involved in processing socially-relevant information.

**Thesis Structure**

The thesis is structured as follows:

- **Chapter 2: Literature Review** – This chapter reviews the existing literature on the neural mechanisms of maternal behavior, the role of oxytocin, and the application of computational methods in neuroscience, particularly TCA.
- **Chapter 3: Theoretical Foundations** – Here, the mathematical framework underlying the methods used in this research, including Tensor Component Analysis and information theory, will be thoroughly discussed.
- **Chapter 4: Experimental Design and Methodology** – This chapter describes the experimental setups used in this study, including the behavioral paradigms and neural recording techniques.
- **Chapter 5: Tensor Component Analysis (TCA) and Neural Dynamics** – The focus here is on the application of TCA to the experimental data, interpreting the neural dynamics revealed through this analysis.
- **Chapter 6: Analysis of Neural Activity and Behavioral Correlates** – This chapter presents a detailed analysis of the spike-train data and effective connectivity, comparing neural activity across different experimental conditions.
- **Chapter 7: Discussion** – The findings are discussed in the context of existing research, with a focus on the implications for computational neuroscience and future research directions.
- **Chapter 8: Conclusion** – The thesis concludes with a summary of the contributions and the broader impact of the research.

# Integration with Current Research

The reviewed literature highlights the increasingly critical role of combining advanced computational methods with invasive and non-invasive neuroscience techniques to dissect complex neural dynamics. Traditional approaches such as PCA and ICA have paved the way for initial explorations of neural patterns, but their limitations in capturing the temporal and interactive nature of neural data necessitate more sophisticated methods like Tensor Component Analysis (TCA). TCA, with its ability to decompose multi-dimensional data into distinct neuron, time, and trial factors, offers a powerful framework for unraveling the intricate neural underpinnings of behavior.

Cichocki et al. (2015) pioneered the application of tensor methods in neuroscience, demonstrating their superiority over matrix factorization techniques in preserving the multi-dimensional structure of the data. Studies by Williams et al. (2018) further expanded on this by applying TCA to large-scale neural recordings, illustrating how this method can identify distinct neural components associated with behavioral states.

Studies on neural synchrony emphasize its importance in cognitive functions, demonstrating that synchronized neural activity correlates with active engagement and efficient learning. The integration of machine learning and recurrent neural network (RNN) architectures further expands our ability to model and predict neural responses based on past activity, complementing the insights gained from TCA. Researchers like Sussillo et al. (2016) demonstrated the utility of RNNs in simulating neural dynamics, revealing that these models can learn complex patterns of neural activity associated with specific tasks.

The application of invasive recording techniques, such as electrode arrays and optogenetics, provides an empirical backbone that supports computational findings. Direct measurement and manipulation of neural circuits, particularly within the PVN/oxytocin system, reveal how specific neuropeptides like oxytocin modulate neural synchrony and connectivity, thus influencing behavior. This biological validation enhances the interpretability of computational results, bridging the gap between theoretical models and real-world neural processes.

The transition from MATLAB to Python further exemplifies the field's drive towards more accessible and efficient data analysis pipelines. Python's open-source ecosystem, with libraries tailored for tensor decomposition, machine learning, and advanced statistical modeling, democratizes access to cutting-edge tools, enabling researchers to replicate and extend findings seamlessly.

**Future Directions and Relevance:** The integration of these methodologies underscores the necessity for a multi-disciplinary approach in modern neuroscience research. By combining computational prowess with rigorous experimental techniques, the field is poised to unlock deeper insights into the neural mechanisms that underpin learning, engagement, and behavior. The subsequent sections will delve into the application of TCA on experimental neural data, presenting detailed analyses that illustrate how neural circuits adapt under varying engagement conditions, and ultimately, contributing to a comprehensive understanding of neural plasticity in complex learning environments.

This integrated approach not only aligns with current research trends but also highlights the potential for these methods to drive future discoveries. The literature reviewed herein serves as a foundation for the advanced analyses that follow, where the application of TCA will illuminate the nuanced interplay between neural synchrony, engagement, and learning, providing valuable contributions to both computational neuroscience and behavioral research.

# Theoretical Foundations

The study of neural mechanisms underlying complex behaviors, such as maternal behavior, requires sophisticated mathematical frameworks capable of decomposing and analyzing high-dimensional neural data. This research employs Tensor Component Analysis (TCA) as a central method for extracting and interpreting latent structures within multi-dimensional datasets. To fully capture the intricacies of neural circuits, including the directional flow of information between neurons, TCA is complemented with concepts from information theory, specifically Transfer Entropy (TE). This section rigorously outlines the mathematical foundations of these techniques, providing the theoretical underpinning for their application in this research.

## Tensor Component Analysis (TCA): Mathematical Foundations

Tensor Component Analysis (TCA) extends the capabilities of Principal Component Analysis (PCA), a commonly used technique for dimensionality reduction in two-dimensional data. While PCA is restricted to analyzing variance in matrices, TCA generalizes this approach to tensors, which are multi-dimensional arrays. This extension allows TCA to handle data that varies across three or more dimensions, such as neurons, time points, and experimental conditions, offering a more comprehensive analysis of complex neural datasets encountered in neuroscience.

### Connection to Principal Component Analysis (PCA)

To appreciate TCA, it is crucial to revisit PCA's mathematical formulation. Given a data matrix $X \in \mathbb{R}^{N \times T}$, where $N$ represents the number of neurons and $T$ denotes time points, PCA seeks to decompose $X$ into the product of three matrices:

$$X = U\Sigma V^\top,$$

where:

- $U \in \mathbb{R}^{N \times R}$ contains the left singular vectors corresponding to the principal components in the neuron space,
- $\Sigma \in \mathbb{R}^{R \times R}$ is a diagonal matrix of singular values representing the variance captured by each component,

- $V \in \mathbb{R}^{T \times R}$ contains the right singular vectors representing principal components in the time domain.

PCA identifies the directions (eigenvectors) that maximize data variance and projects the data onto these directions, reducing dimensionality while preserving the data's primary variance structure. However, PCA's limitation to two dimensions restricts its application in neuroscience, where data often extends into multiple dimensions, including neurons, time, and experimental conditions. TCA addresses this by extending the decomposition to tensors.

## Tensor Component Analysis (TCA): Generalization to Higher Dimensions

TCA generalizes PCA by decomposing tensors—multi-dimensional arrays—into factor matrices and scalar weights. Consider a tensor $\mathcal{X} \in \mathbb{R}^{N \times T \times K}$, representing data across neurons ($N$), time points ($T$), and trials or conditions ($K$). TCA decomposes this tensor as a sum of rank-one tensors:

$$\mathcal{X}_{i,j,k} \approx \sum_{r=1}^{R} \lambda_r \mathbf{a}_{i,r} \mathbf{b}_{j,r} \mathbf{c}_{k,r},$$

where:

- $\lambda_r$ are scalar weights,
- $\mathbf{a}_r \in \mathbb{R}^N$ are factor vectors corresponding to neurons,
- $\mathbf{b}_r \in \mathbb{R}^T$ are factor vectors corresponding to time points,
- $\mathbf{c}_r \in \mathbb{R}^K$ are factor vectors corresponding to trials or conditions.

TCA decomposes data across multiple dimensions, capturing interactions and patterns not discernible through PCA. This decomposition is essential for analyzing the intricate relationships between neural activity, temporal dynamics, and varying experimental conditions.

## Optimization Problem and Tensor Decomposition

The TCA optimization problem seeks to minimize the reconstruction error between the original tensor $\mathcal{X}$ and its rank-one approximation:

$$\min_{\mathbf{A},\mathbf{B},\mathbf{C},\lambda_r} \left\| \mathcal{X} - \sum_{r=1}^{R} \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r \right\|_F^2,$$

subject to:

$$\|\mathcal{X}\|_F = \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{T} \sum_{k=1}^{K} |\mathcal{X}_{i,j,k}|^2},$$

where $\| \cdot \|_F$ denotes the Frobenius norm, a generalization of the Euclidean norm to tensors.

This non-convex optimization problem is typically approached using Alternating Least Squares (ALS), which iteratively optimizes each factor matrix while holding the others fixed. The process repeats until convergence, providing an efficient means to decompose complex, multi-dimensional data.

## Role of Kronecker and Khatri-Rao Products

The Kronecker and Khatri-Rao products are instrumental in TCA, particularly in the tensor unfolding and optimization processes.

The **Kronecker product** $A \otimes B$ between matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$ is defined as:

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix} \in \mathbb{R}^{mp \times nq},$$

which expands matrices, aiding in tensor unfolding.

The **Khatri-Rao product**, a column-wise Kronecker product, simplifies the optimization problem by efficiently combining factor matrices:

$$A \odot B = [\mathbf{a}_1 \otimes \mathbf{b}_1 \ \mathbf{a}_2 \otimes \mathbf{b}_2 \ \dots \ \mathbf{a}_r \otimes \mathbf{b}_r] \in \mathbb{R}^{mn \times r}.$$

These products facilitate the transformation of tensors into matrix forms suitable for optimization, enhancing the computational efficiency of TCA.

## Tensor Unfolding and Mode-n Products

Unfolding, or matricization, reconfigures a tensor into a matrix, crucial for implementing TCA. For a tensor $\mathcal{X} \in \mathbb{R}^{N \times T \times K}$, unfolding along different modes yields

matrices such as:

- Mode-1 unfolding: $\mathcal{X}_{(1)}$ with size $N \times (T \times K)$,
- Mode-2 unfolding: $\mathcal{X}_{(2)}$ with size $T \times (N \times K)$,
- Mode-3 unfolding: $\mathcal{X}_{(3)}$ with size $K \times (N \times T)$.

The **mode-n product** of a tensor $\mathcal{X}$ with a matrix $A \in \mathbb{R}^{M \times N_n}$ along the $n$-th mode, denoted as $\mathcal{Y} = \mathcal{X} \times_n A$, modifies the tensor along a specific dimension, playing a key role in the decomposition process.

### Tucker and CP Decompositions

TCA is closely linked to Tucker and Canonical Polyadic (CP) decompositions:

- **Tucker Decomposition** generalizes PCA by decomposing a tensor into a core tensor $\mathcal{G}$ and factor matrices:

$$\mathcal{X} \approx \mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C},$$

  allowing interaction between components in different modes.

- **CP Decomposition**, a special case of Tucker decomposition, simplifies to a sum of rank-one tensors when the core tensor is diagonal.

These decompositions provide powerful tools for multi-way data analysis, extracting meaningful patterns from complex neural recordings.

## Transfer Entropy: Quantifying Effective Connectivity

While TCA captures latent structures in neural data, it does not address the causal interactions between neurons. To quantify these directional influences, Transfer Entropy (TE) is employed as a measure of effective connectivity. TE evaluates the amount of information transferred from

one neuron to another, considering the temporal sequences of their activities.

Given time series $X_t$ and $Y_t$ representing neuron activities, TE from $X$ to $Y$ is defined as:

$$TE_{X\to Y} = \sum_{x_t, y_{t+1}, y_t} p(y_{t+1}, y_t, x_t) \log \frac{p(y_{t+1} \mid y_t, x_t)}{p(y_{t+1} \mid y_t)},$$

which quantifies how much the state of $X$ reduces the uncertainty of $Y$'s future state beyond what $Y$'s past alone can explain.

## Estimation of Probability Distributions

Estimating the joint and conditional probabilities $p(y_{t+1}, y_t, x_t)$, $p(y_{t+1} \mid y_t, x_t)$, and $p(y_{t+1} \mid y_t)$ is critical for computing TE. Techniques such as Kernel Density Estimation (KDE) or model-based approaches like Generalized Linear Models (GLM) and Autoregressive (AR) models are often used.

KDE estimates the probability density function from data points $\{x_i\}_{i=1}^n$ using:

$$\hat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right),$$

where $K(u)$ is typically a Gaussian kernel, and $h$ controls the smoothness. This method is particularly useful for estimating the probability densities needed for TE calculations from spike trains or continuous neural data.

Alternatively, GLM can be employed to model the influence of past neuron states on current firing rates, providing estimates for TE computation. For example, a Poisson GLM for spike count data can be formulated as:

$$\log \lambda(t) = \beta_0 + \sum_{k=1}^{p} \beta_k X_{t-k},$$

where $\lambda(t)$ is the expected firing rate at time $t$, allowing the estimation of the conditional distributions used in TE.

## Visualization of Transfer Entropy Results

The results of TE analysis are typically visualized as directed graphs or matrices, where nodes represent neurons and edges denote the direction and strength of information transfer. This approach provides a visual summary of the effective connectivity within neural circuits, highlighting the pathways through which neurons influence each other during learning.

The integration of TCA and TE thus provides a robust framework for dissecting neural dynamics, capturing both structural patterns and causal interactions

within neural circuits.

# Experimental Design and Methodology

## Experimental Design

The neural basis of social learning in mammals, particularly how naive individuals acquire complex social behaviors, remains a key challenge in neuroscience. This study investigates the mechanisms by which naive virgin mice acquire pup-retrieval behavior—a critical aspect of maternal care—through the observation of experienced mother mice (dams). The primary objective is to identify and characterize the neural circuits and plasticity mechanisms within the paraventricular nucleus (PVN) of the hypothalamus that facilitate this form of social learning.

### Hypothesis

We hypothesize that naive virgin mice can acquire pup-retrieval behavior through social observation of experienced dams. This learning process is expected to involve significant changes in neural activity patterns and connectivity within the PVN, particularly those mediated by oxytocinergic signaling pathways. By investigating the dynamics of PVN activity, we aim to elucidate the functional reorganization of this region's circuitry, which drives the transition from a naive state to one capable of executing learned maternal behaviors.

### Subjects and Experimental Groups

Three distinct groups of adult female C57BL/6J mice were employed in this study to create a comprehensive social learning model:

- **Naive Virgin Mice:** Female mice without prior exposure to pups or maternal care serve as the primary subjects to examine the neural underpinnings of learning parenting behaviors.
- **Dams:** These are experienced mother mice that have been previously conditioned in pup-retrieval. Dams perform the pup-retrieval task, serving as demonstrators for naive virgin mice to observe and learn from.
- **Isolated Pups:** Pups (postnatal day 4-6) are utilized to evoke natural pup-retrieval behaviors from the dams, thereby providing a dynamic social stimulus

for the learning paradigm.

## Experimental Setup Illustration

To provide a clear visual representation of the experimental setup, **Figure 1** shows the different contexts of social behavior, including isolated pups, dams, and naive virgin mice. This figure highlights the roles and interactions among the different groups in the social learning paradigm.

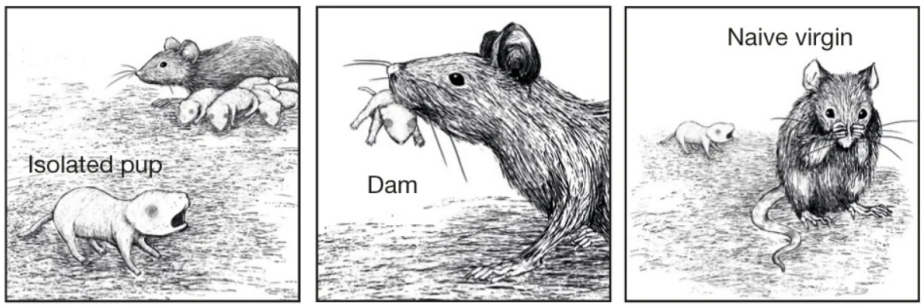


Figure 1: Illustration of the experimental setup: (Left) An isolated pup serves as a stimulus for dams to perform pup-retrieval. (Center) Dam mouse retrieving a pup, demonstrating maternal behavior. (Right) Naive virgin mouse observing the dam's behavior to learn pup-retrieval.

## Social Learning Paradigm

The experimental paradigm centers around a *social observational learning task* where naive virgin mice observe dams retrieving isolated pups. Two distinct regimes were employed to dissect both passive observation and active engagement in the learning process:

1. **Passive Observational Learning Regime:** In this regime, head-fixed naive virgin mice were exposed to video recordings of dams retrieving isolated pups. The recordings encompassed multiple trials, capturing various phases of pup retrieval (e.g., approaching the pup, picking up the pup, and returning to the nest), allowing the naive mice to observe the complete sequence of maternal behaviors. The videos were presented at regular intervals to ensure consistent exposure while the neural activity of the observing mice was continuously recorded. As shown on the left side of **Figure 2**, the mice watched the videos passively without any control over the playback.

2. **Active Engagement Learning Regime:** In this setup, naive virgin mice were given the opportunity to actively participate in the learning process by interacting with the environment. The mice were head-fixed and trained to press a lever to initiate the playback of pup-retrieval videos. This design allows the mice to exercise agency, making a conscious decision to engage with the socially relevant stimuli rather than passively observing the behavior (as shown on the right side of **Figure 2**).

   The lever-pressing task serves as a measure of the mouse's motivation to learn the pup-retrieval behavior, providing a more dynamic and interactive form of social learning. By requiring the mice to press a lever to view each instance of pup-retrieval behavior by a dam, this regime tested whether such active engagement enhances learning efficacy. Specifically, it investigates how neural circuits involved in motivation and reward processing interact with social learning circuits within the PVN.

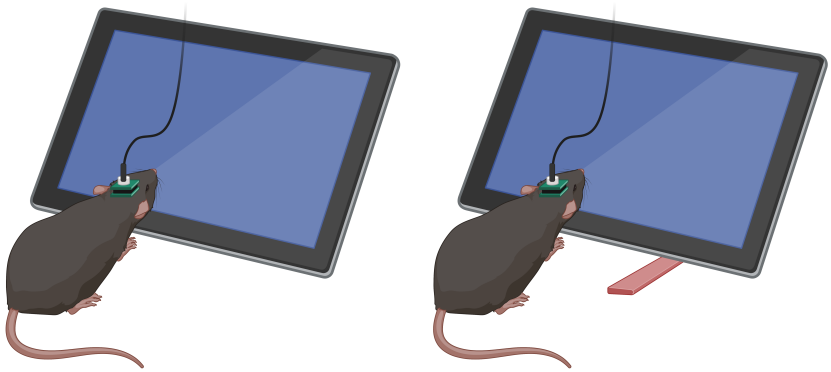

Figure 2: Illustration of two learning regimes for naive virgin mice watching pup-retrieval videos. (Left) Passive learning regime where the mouse is head-fixed and observes the video without control over playback. (Right) Active engagement learning regime where the mouse must press a lever to initiate playback, providing an interactive component to the social learning process.

## Neural Recording and Experimental Conditions

Neural recordings were conducted to capture PVN activity using high-density silicon probes (Buzsaki32L; see **Figure 3**). The PVN was specifically targeted due to

its established role in modulating oxytocin release and regulating social behaviors. Recordings were performed in head-fixed mice under both passive and active learning conditions, allowing for simultaneous monitoring of large neural populations to capture both single-unit and network-level dynamics throughout the learning process.

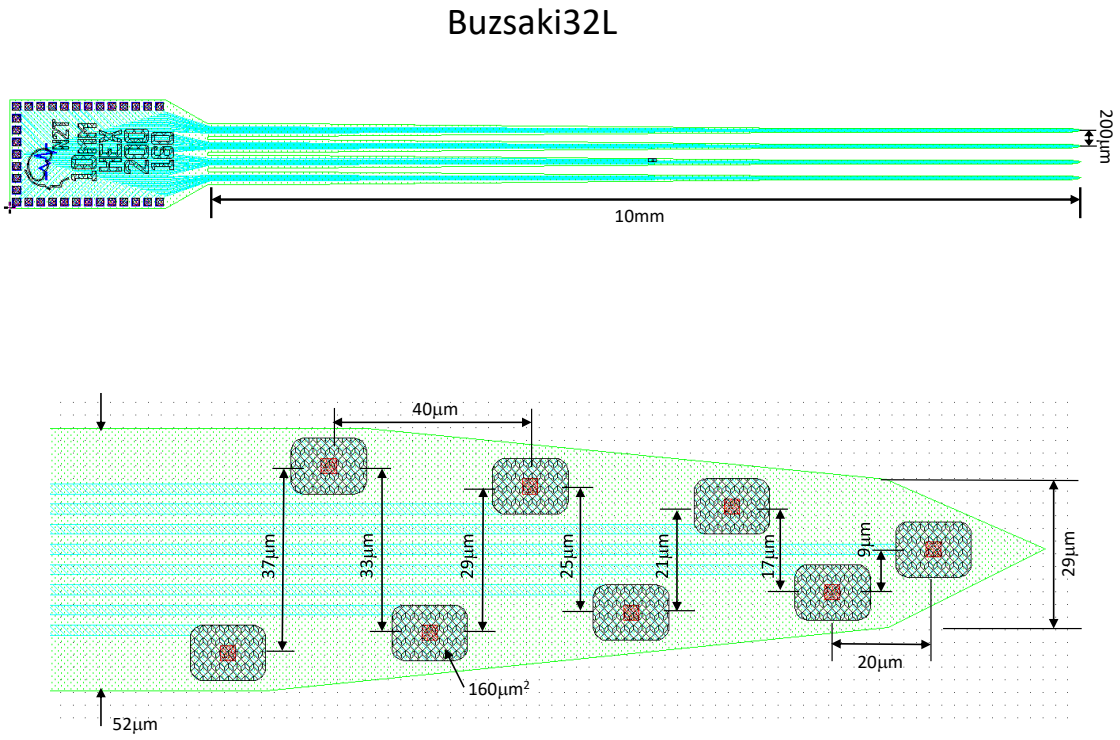


Figure 3: Neural recording setup using high-density silicon probes targeting the PVN.

## Behavioral and Neural Correlates

Following the observation sessions, behavioral performance was assessed by allowing the naive virgin mice to perform the pup-retrieval task in a controlled environment. Neural correlates of learning, such as changes in firing rates, spike timing, and network connectivity within the PVN, were analyzed to elucidate the underlying mechanisms of acquired maternal behaviors.

# Methodology

## Animal Preparation and Surgical Procedures

All experimental procedures were approved by the Institutional Animal Care and Use Committee (IACUC) and adhered to NIH guidelines for the care and use of laboratory animals. Female mice (8-10 weeks old) were anesthetized using isoflurane (2-3% induction, 1-2% maintenance), and a custom-designed titanium headplate was surgically affixed to the skull using dental cement. The mice were allowed to recover for 5-7 days before electrophysiological recordings commenced.

For *in vivo* recordings, a Buzsaki32L silicon probe was stereotaxically implanted into the PVN (coordinates: AP -0.82 mm, ML $\pm$0.1 mm, DV -4.8 mm) with reference to bregma. The probe targets oxytocinergic neurons involved in maternal behaviors, with 32 recording sites spaced at 40 $\mu$m intervals, enabling high-resolution monitoring of local field potentials and spiking activity. Electrode placements were verified post-experiment through histological staining and imaging.

## Electrophysiological Recording and Spike Sorting

Electrophysiological signals were amplified, bandpass filtered (300-6000 Hz for spikes), and digitized at 30 kHz using an Open Ephys acquisition system. Spike sorting was performed using Kilosort2, followed by manual curation with Phy to ensure high-quality spike clusters representing individual neurons. Cluster quality was validated using metrics such as isolation distance, L-ratio, and refractory period violations, ensuring that recorded spikes were from well-isolated single units.

## Data Analysis: Spike Times and Firing Patterns

To decode the neural activity underlying the learning of parenting behavior in naive virgin mice, a comprehensive analysis of spike times and firing patterns was performed. This analysis aimed to understand how the paraventricular nucleus (PVN) dynamically processes social information and how these patterns change during the learning process.

### Waveform Extraction and Classification

Neural signals were recorded at a high temporal resolution (30 kHz sampling rate), allowing for the capture of extracellular action potentials, or "spikes," from indi-

vidual neurons. The raw electrophysiological recordings were processed to extract spike waveforms, providing essential information about the underlying neural activity. These waveforms were carefully sorted into clusters corresponding to putative single neurons based on features such as amplitude, shape, and duration.

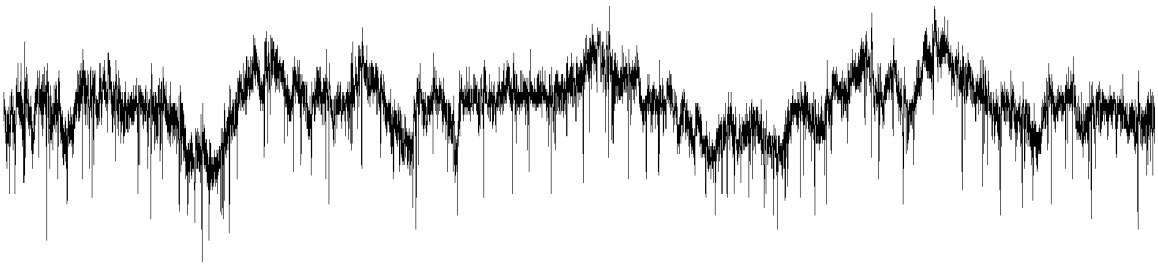

Figure 4: Visualization of extracted spike waveforms recorded from the PVN, showcasing distinct neuronal types and firing properties.

### Spike Raster Plots and Peristimulus Time Histograms (PSTHs)

After spike sorting, spike times were plotted in *spike raster plots*, which depict the spiking activity of each neuron over multiple trials. Raster plots provide a visual representation of the timing and variability of spikes across trials, revealing the temporal coordination of neural firing in response to the presentation of pup-retrieval videos. For each trial, spikes were binned in 1 ms intervals to ensure precise temporal resolution, revealing both synchronous and asynchronous firing patterns across the PVN network.

**PSTHs Calculation:** To quantify changes in firing rates, *Peristimulus Time Histograms (PSTHs)* were generated for each neuron across all trials (see **Figure 5**). PSTHs were computed by binning spike counts into 50 ms bins around the onset of pup-retrieval videos and normalizing them to the baseline firing rates observed during pre-stimulus periods. The resulting PSTHs were z-scored to facilitate comparison across neurons and conditions, emphasizing significant excitatory and inhibitory responses relative to baseline activity.

### Identification of Socially Relevant Neural Responses

As depicted in **Figure 5**, several neurons demonstrated stereotypical patterns of activity aligned with specific moments in the pup-retrieval task, such as the dam approaching, picking up, and returning the pup. These time-locked patterns suggest

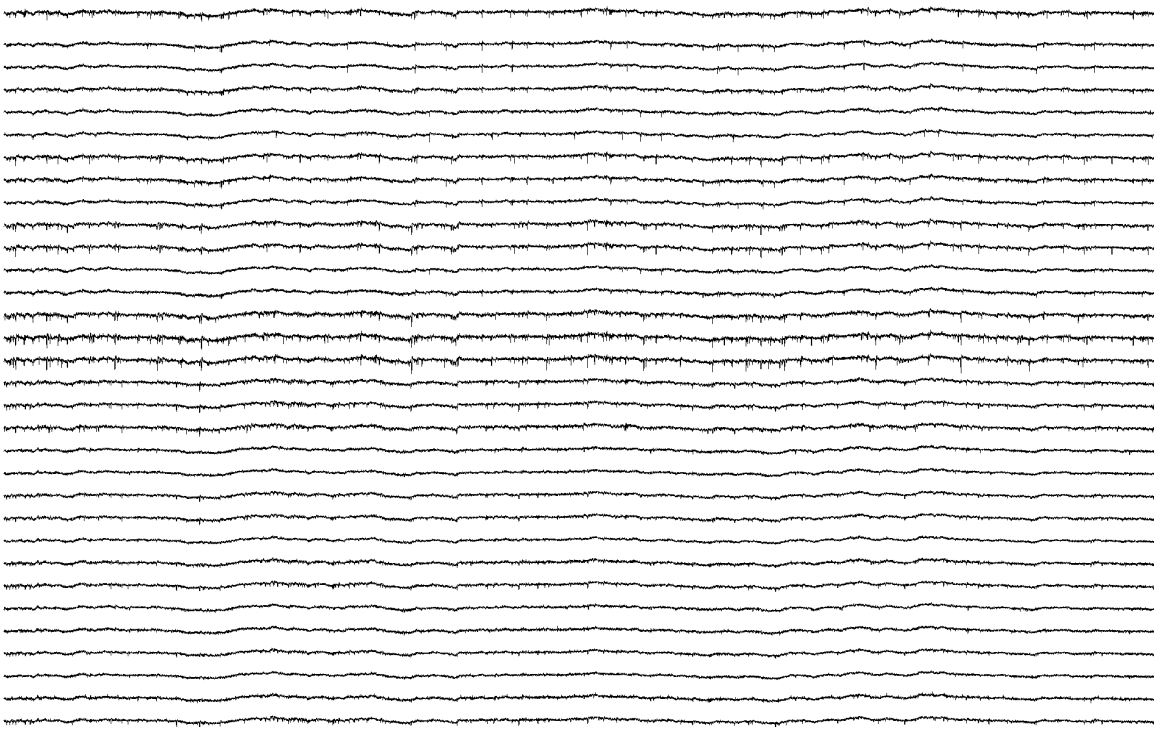

Figure 5: Peristimulus Time Histograms (PSTHs) generated for each neuron across all trials, normalized to baseline firing rates.

that the PVN not only processes visual cues related to pup presence but also encodes the sequence of actions performed by the dam. Such encoding is hypothesized to be critical for naive virgin mice to learn the behavioral sequence needed for effective pup retrieval.

### Waveform and Firing Rate Dynamics Across Conditions

By overlaying the extracted spike waveforms with the spike raster plots and Peristimulus Time Histograms (PSTHs), we obtained a multi-dimensional view of how different neuronal subpopulations within the PVN are engaged during the learning process. Raster plots depict the precise timing of spikes across multiple neurons and trials, providing an overview of population activity and temporal coordination in response to behavioral events, such as the start of a pup-retrieval video (see **Figure 7**).

Distinct firing rate patterns, as shown in **Figures 6** and **7**, revealed both excitatory bursts and periods of suppression that correlate with key behavioral events observed during the pup-retrieval videos. The combination of these visualizations allows us to identify neurons that show significant modulation in their activity in

response to the observed social stimuli, such as an increase in firing rate when the dam approaches or retrieves a pup. This method provides insight into the dynamic changes in neural activity that are hypothesized to underlie learning of the pup-retrieval behavior by naive virgin mice.

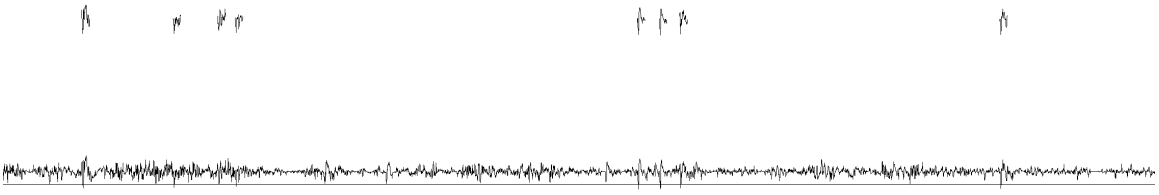

Figure 6: Dynamics of neural activity within the PVN showing distinct firing rate patterns in response to pup-retrieval events.

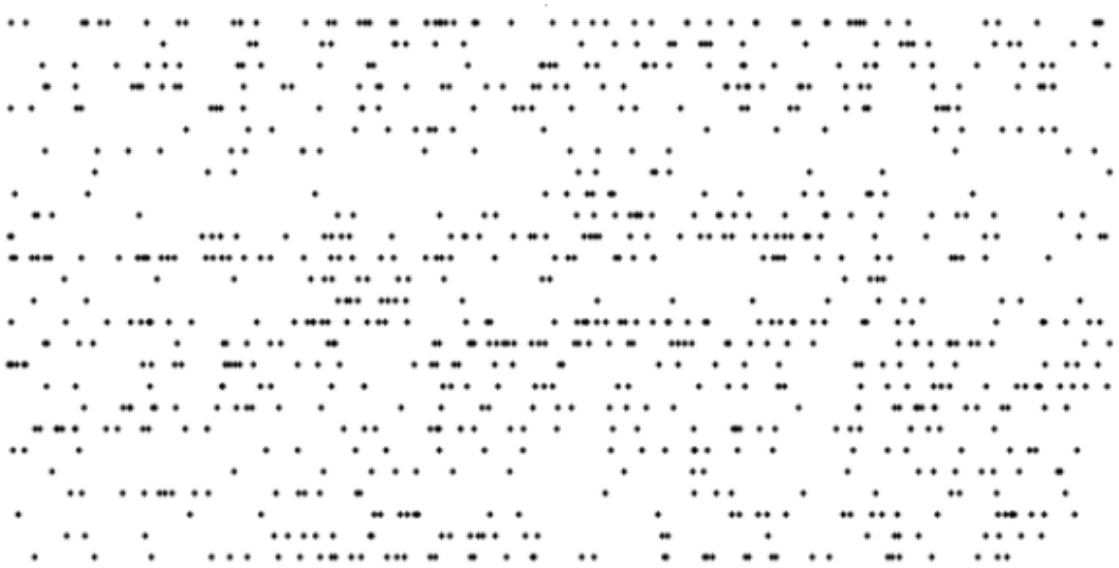

Figure 7: Spike raster plots showing the timing of spikes across multiple neurons and trials, aligned to the onset of pup-retrieval videos (indicated by the "video start" marker). These plots provide a comprehensive view of neural population activity during the social learning task.

## Tensor Component Analysis (TCA)

To investigate the neural dynamics underlying the learning of pup-retrieval behavior in naive virgin mice, we employed Tensor Component Analysis (TCA). TCA is a

powerful dimensionality reduction technique that is well-suited for high-dimensional neural data, as it allows for the decomposition of multi-way data structures (tensors) into low-dimensional components that capture essential features of neural activity patterns across neurons, time, and trials. This section outlines the preparation and preprocessing steps involved in constructing the data tensor for TCA, which serves as the basis for subsequent analysis.

### Construction of the Spike Count Tensor

The raw electrophysiological data, consisting of spike trains recorded from multiple neurons within the paraventricular nucleus (PVN), were preprocessed to generate a three-dimensional tensor $X \in \mathbb{R}^{N \times T \times M}$. Here, $N$ denotes the number of neurons recorded, $T$ represents the number of time bins, and $M$ corresponds to the number of trials. Each element $X_{n,t,m}$ in the tensor represents the spike count or z-scored firing rate of neuron $n$ in time bin $t$ during trial $m$.

Prior to constructing the tensor, the spike trains were binned into discrete time windows to create spike counts for each neuron across trials. The choice of bin size ($\Delta t$) was optimized to balance temporal resolution and noise reduction, ensuring meaningful representation of neural dynamics. Following binning, spike counts were normalized using z-scoring to account for variability in firing rates across neurons, thereby facilitating comparison across different neurons and experimental conditions.

### Preparation for TCA Decomposition

The prepared tensor $X$ was then used as input for TCA to decompose it into a sum of rank-1 tensors. Specifically, TCA aims to find a low-rank approximation of the form:

$$X \approx \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r,$$

where $R$ is the number of components, and $\mathbf{a}_r \in \mathbb{R}^N$, $\mathbf{b}_r \in \mathbb{R}^T$, and $\mathbf{c}_r \in \mathbb{R}^M$ are vectors that represent the factors for neurons, time, and trials, respectively, for the $r$-th component. The symbol $\circ$ denotes the outer product, which allows the decomposition to capture the interactions across the three dimensions.

### Interpretation of TCA Components

Each component extracted from the TCA decomposition provides a mode of variation that is interpretable within the context of the neural data:

- **Neuronal Components** ($\mathbf{a}_r$): Represent groups of neurons that exhibit correlated activity patterns across trials. These components can reveal functional subnetworks within the PVN that are co-activated during specific stages of the learning process.
- **Temporal Components** ($\mathbf{b}_r$): Capture temporal patterns of neural activity that evolve over time, such as responses to distinct phases of the pup-retrieval behavior (e.g., onset of observation, approach to the pup, retrieval). These components provide insight into how neural circuits are dynamically modulated in response to behavioral stimuli.
- **Trial Components** ($\mathbf{c}_r$): Describe variability or consistency in neural responses across trials, allowing differentiation between stable neural patterns and trial-specific effects that may reflect variability in behavior or context.

### Data Preparation for Further Analysis

The extracted TCA components ($\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r$) serve as the basis for subsequent analyses aimed at understanding the neural encoding of socially relevant information and the mechanisms of learning and adaptation. Further data processing steps, including clustering of TCA components to identify functionally relevant groups, assessment of component stability across sessions, and correlation of neural components with behavioral performance metrics, will be detailed in the TCA implementation section. These steps provide a comprehensive understanding of how neural circuits within the PVN support the acquisition of complex social behaviors.

# Implementation of TCA on Neuron Firing Data

## Introduction

The initial step in implementing Tensor Component Analysis (TCA) on neural data involves the preparation and preprocessing of spike-train data obtained from electrophysiological recordings. Neural firing data are typically stored in formats that contain raw spike timestamps, cluster assignments, and quality metrics for each neuron cluster. These datasets are imported into a computational environment for further processing to transform continuous spike times into a structured format suitable for tensor-based analysis. Preprocessing consists of several essential steps: filtering neurons based on quality labels and firing rate thresholds, discretizing continuous spike times into defined time bins to compute firing rates, and organizing the resulting data into a multi-dimensional tensor format. This tensor format is designed to capture the dynamics of neural activity across time, trials, and neuronal populations, providing a robust foundation for subsequent analysis using TCA. Each step in the preprocessing pipeline is crucial to ensure that the data is of high quality and is appropriately formatted for extracting meaningful patterns in neural activity.

## Data Preparation and Preprocessing

The initial step in implementing TCA on neural data is the preparation and preprocessing of spike-train data obtained from electrophysiological recordings. The neural firing data is stored in `.npy` and `.tsv` files, which are loaded into MATLAB for further processing.

### Spike Data Acquisition and Filtering

Neural spike data are represented by two arrays: `spike_times.npy`, which contains the timestamps of spikes, and `spike_clusters.npy`, which contains cluster IDs that map each spike to a specific neuron. These files are loaded into MATLAB using the `readNPY` function (Listing 1).

```
spikeTimes = double(readNPY(fullfile(expF, 'spike_times.npy')));
spikeClusters = readNPY(fullfile(expF, 'spike_clusters.npy'));
```

Listing 1: Loading Spike Times and Clusters

The spike times, stored in the variable `spikeTimes`, are recorded at a high sampling frequency of 30,000 Hz, providing a high temporal resolution for spike events. The cluster IDs, stored in the variable `spikeClusters`, map each spike to a corresponding neuron ID, allowing for the analysis of spike trains for individual neurons (Listing 2).

```
% Read the cluster group data from the TSV file
clusterGroupStruct = tdfread(fullfile(expF, 'cluster_group.tsv'), '\
    t');

% Extract cluster IDs and group labels
clusterID = clusterGroupStruct.cluster_id;
clusterGroup = string(clusterGroupStruct.group);
```

Listing 2: Reading and Processing Cluster Group Data

Quality information for each cluster is provided in `cluster_group.tsv`, which tags each cluster as *good* (single-unit activity), *MUA* (multi-unit activity), or *noise*. Neurons labeled as *noise* are excluded from the analysis, while *good* neurons are always included. If `includeMUA` is set to `true`, neurons labeled as *MUA* are also included. This filtering is critical to ensure that only high-quality, reliable signals are analyzed, thereby minimizing noise and maximizing the accuracy of the results (Listing 3).

```
% Determine the number of 'good' and 'mua' clusters
numGoodClusters = sum(strcmp(clusterGroup, 'good'));
numMUAClusters = sum(strcmp(clusterGroup, 'mua'));

% Initialize the array for good clusters based on inclusion criteria
if includeMUA
    goodClustID = zeros(numGoodClusters + numMUAClusters, 1);
else
    goodClustID = zeros(numGoodClusters, 1);
end
```

Listing 3: Filtering Neurons Based on Criteria

Additionally, neurons with a minimal firing rate below a defined threshold (e.g., 0.1 Hz) are excluded from analysis to ensure only neurons with sufficient activity levels contribute to the tensor construction.

## Construction of the Spike-Train Tensor

The spike-train data is transformed into a three-dimensional tensor $\mathcal{A}$ with dimensions corresponding to neurons ($N$), time bins ($T$), and trials ($K$). Each element $A_{n,t,k}$ represents the spike count of neuron $n$ within time bin $t$ during trial $k$. This tensor format is crucial for capturing the temporal dynamics of neural activity across multiple trials.

**Discretizing Spike Times into Time Bins:** The continuous spike times are converted into discrete time bins to compute spike counts. The time window around each stimulus is defined by the parameter `straddleTime` (e.g., -5 to +10 seconds around stimulus onset), and the temporal resolution of the bins is controlled by the parameter `binSize` (e.g., 1/3 second). A smaller bin size offers higher temporal resolution but may lead to increased variability due to low spike counts, while a larger bin size provides smoother estimates of firing rates (Listing 4).

```
% Define the time window around the stimulus and the bin size
straddleTime = 10;  % Time window (in seconds) around the stimulus
binSize = 1/3;      % Time bin size (in seconds)

% Calculate the total number of bins for the defined time window and
    bin size
binCount = int32((2 * straddleTime) / binSize);
```

Listing 4: Discretizing Spike Times into Time Bins

**Building the Spike-Train Tensor:** For each neuron and trial, the spike times are centered on stimulus onsets (`flagTimes`), binned using `histcounts` to compute spike counts, and stored in tensor $\mathcal{A}$. This structured format is essential for TCA, as it allows for the identification of neural patterns across time, trials, and neuronal populations (Listing 5).

```
% Iterate over each neuron to construct the spike-train tensor
for neuronIdx = 1:length(goodClustID)

    % Extract spike times for the current neuron
    spikeTimesCluster = spikeTimes(spikeClusters == goodClustID(
   neuronIdx)) / samplingFreq;  % Convert to seconds

    % Initialize an array to store binned spike counts for the
   current neuron
    binnedSpikeCounts = zeros(1, binCount);

```

```
    % Bin the spikes for each trial and store in the tensor
    for trialIdx = 1:numTrials
        % Bin the spikes for the current trial
        binnedSpikeCounts = histcounts(spikeTimesCluster, binEdges);

        % Store the Z-scored firing rates in the tensor
        NTK(neuronIdx, :, trialIdx) = zscore(binnedSpikeCounts);
    end
end
```

Listing 5: Building the Spike-Train Tensor

# Normalization and Smoothing of Data

## Z-Score Normalization of Firing Rates

To facilitate meaningful comparisons across neurons, Z-score normalization is applied to the firing rates. This standardization step centers the data around zero and scales it by the standard deviation of firing rates during the pre-stimulus period, effectively removing baseline differences between neurons and allowing for the identification of stimulus-related changes in firing patterns

$$Z_{n,t,k} = \frac{R_{n,t,k} - \mu_n^{\text{pre}}}{\sigma_n^{\text{pre}}},$$

where $\mu_n^{\text{pre}}$ and $\sigma_n^{\text{pre}}$ are the mean and standard deviation of firing rates during the pre-stimulus period:

$$\mu_n^{\text{pre}} = \frac{1}{T^{\text{pre}}} \sum_{t=1}^{T^{\text{pre}}} R_{n,t,k}, \quad \sigma_n^{\text{pre}} = \sqrt{\frac{1}{T^{\text{pre}}} \sum_{t=1}^{T^{\text{pre}}} (R_{n,t,k} - \mu_n^{\text{pre}})^2}.$$

The Z-scored data are then stored in a new tensor $\mathcal{Z}$.

## Gaussian Smoothing for Noise Reduction

Gaussian smoothing is subsequently applied to the Z-scored data to reduce noise and highlight broader temporal patterns in neural activity. This step is particularly useful for visualizing Peri-Stimulus Time Histograms (PSTHs) and capturing consistent trends in the data, enhancing the interpretability of the results (Listing 6).

```
% Apply Gaussian smoothing to the firing rates using a specified
    kernel size
kernelSize = 5;  % Define the size of the Gaussian kernel
flagSpecificFiringRates_smooth = smoothdata(flagSpecificFiringRates,
    'gaussian', kernelSize);
```

Listing 6: Applying Gaussian Smoothing

## Visualization of Neural Activity and Peri-Stimulus Time Histograms (PSTHs)

To illustrate the impact of preprocessing steps such as normalization and smoothing, we present visualizations of neural activity from a specific neuron cluster (neuron_179). Figure 8 includes three panels that provide different perspectives on the neural responses during trials. The top panel shows a raster plot of spikes across trials, where each dot represents a spike and each row represents a trial. This visualization captures the precise timing of spikes relative to the video onset. The middle panel displays the average firing rate over time, indicating the overall neural activity trends across trials and highlighting periods of increased or decreased firing. The bottom panel shows the deviation from the average firing rate, providing a clearer view of how the neural response deviates from the baseline activity, which can be useful for identifying significant shifts in firing patterns linked to specific behavioral events.

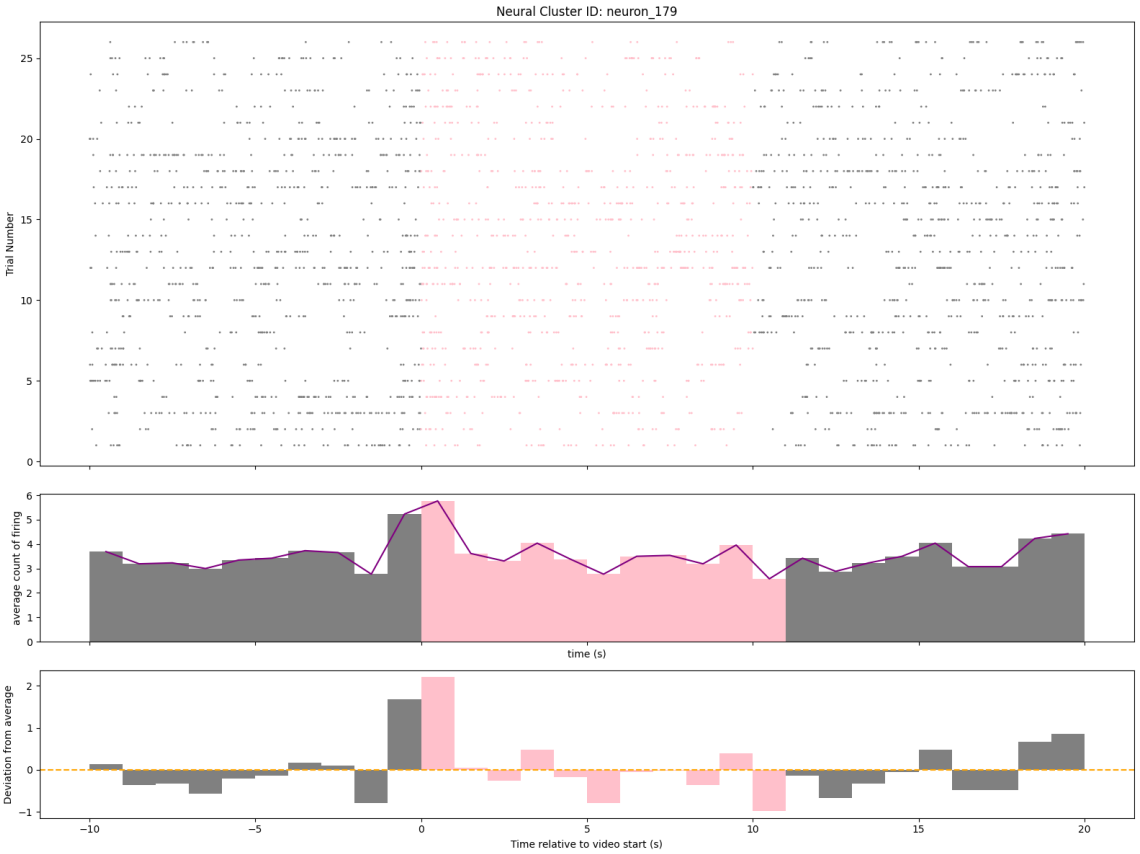


Figure 8: Neural activity visualization for neuron cluster ID: neuron_179. The top panel shows the raster plot of spikes across trials, capturing the timing of individual spikes. The middle panel represents the average firing rate across time, highlighting overall trends in neural activity. The bottom panel depicts the deviation from the average firing pattern relative to video onset, illustrating significant changes in firing rates.

## Scaling for TCA

While the Z-scored data can be directly used for TCA, an optional scaling step to normalize the data to a range of [0, 1] could be applied to prevent any single neuron from dominating the TCA decomposition. This scaling ensures that all neurons contribute equally to the analysis, maintaining the relative differences between data points.

$$S_{n,t,k} = \frac{Z_{n,t,k} - \min(Z_n)}{\max(Z_n) - \min(Z_n)},$$

where $\min(Z_n)$ and $\max(Z_n)$ are the minimum and maximum values of the Z-scored firing rates for neuron $n$. This ensures that all neurons contribute equally

to the TCA.

# Tensor Component Analysis (TCA) Implementation

## Applying TCA Using Alternating Least Squares (ALS)

TCA is implemented using the CANDECOMP/PARAFAC (CP) decomposition model with the Alternating Least Squares (ALS) method. This approach is suitable for decomposing tensors where the data can take on positive and negative values, providing a flexible framework for analyzing complex neural datasets. Alternatively, for data that is inherently non-negative, such as neural firing rates, a Non-Negative CP (NCP) decomposition is more appropriate, imposing non-negativity constraints on the factor matrices to ensure that all components are interpretable in the context of neural activity.

The ALS algorithm (Listing 7) iteratively updates factor matrices to minimize the Frobenius norm of the difference between the original and approximated tensors:

$$\text{minimize} \quad \|\mathcal{A} - \hat{\mathcal{A}}\|_F^2,$$

where the decomposition is given by:

$$\hat{\mathcal{A}} = \sum_{r=1}^{R} \mathbf{w}_r \circ \mathbf{b}_r \circ \mathbf{a}_r.$$

```
% Perform TCA decomposition using Alternating Least Squares (ALS)
numComponents = R;  % Number of components for TCA
model_Z = cp_als(NTK_ten, numComponents, 'printitn', 0);

% Compute the reconstruction error of the TCA model
reconstructedTensor = full(model_Z);
reconstructionError = norm(reconstructedTensor - full(NTK_ten)) /
    norm(NTK_ten);
```

Listing 7: TCA Using Alternating Least Squares (ALS)

The Non-Negative CP (NCP) decomposition (Listing 8) imposes non-negativity constraints on the factor matrices:

$$\text{minimize} \quad \|\mathcal{A} - \hat{\mathcal{A}}\|_F^2, \quad \text{subject to } \mathbf{w}_r, \mathbf{b}_r, \mathbf{a}_r \geq 0.$$

```
% Perform Non-Negative CP (NCP) decomposition on the smoothed tensor
numComponents = R;  % Number of components for NCP
model_Z_smooth = ncp(NTK_smooth, numComponents, 'verbose', 0);
```

Listing 8: Non-Negative Tensor Component Analysis (NCP)

### Parameter Selection and Optimization

Selecting the optimal number of components $R$ is crucial for balancing underfitting and overfitting in the model. The choice of $R$ can be guided by cross-validation, where the dataset is divided into training and validation sets. By iteratively adjusting the rank $R$, the model aims to minimize reconstruction error on unseen data, thereby ensuring generalizability and preventing overfitting.

Regularization techniques, such as L2 regularization, can be applied to control overfitting by penalizing the magnitude of the factor matrices. The objective function with L2 regularization is given by:

$$\text{minimize} \, \|A - \hat{A}\|^2 + \lambda(\|W\|^2 + \|B\|^2 + \|C\|^2),$$

where $\lambda$ is the regularization parameter, and $W$, $B$, and $C$ represent the factor matrices corresponding to different modes (e.g., neurons, time bins, and trials) in the tensor decomposition. Here, $\|A-\hat{A}\|^2$ represents the Frobenius norm of the difference between the original tensor $A$ and its approximation $\hat{A}$, and $\|W\|^2 + \|B\|^2 + \|C\|^2$ are the L2 norms of the factor matrices. The parameter $\lambda$ controls the strength of the regularization, with higher values leading to more regularized, simpler models.

## Conclusion

This section has provided a detailed and thorough guide for implementing Tensor Component Analysis (TCA) on neural firing data using MATLAB. By decomposing high-dimensional neural data into interpretable components, TCA enables researchers to uncover patterns of neural activity associated with different behavioral conditions. This approach offers a powerful framework for advancing our understanding of brain function and the neural basis of behavior. Future work could explore integrating TCA with other machine learning approaches, such as supervised learning methods, to link neural activity patterns more directly with behavioral outputs or experimental conditions.

# Advanced Analysis of Neural Dynamics Using TCA

## Introduction

This chapter provides an in-depth analysis of the neural dynamics underlying active and passive engagement conditions in mice, focusing on data obtained from the hypothalamic paraventricular nucleus (PVN). The PVN is a critical region involved in coordinating complex behaviors, and its activity patterns provide valuable insights into how different behavioral states are encoded by neural circuits. Using Tensor Component Analysis (TCA), we decompose high-dimensional neural data into neuron-specific, temporal, and trial-specific components to uncover distinct patterns of neural engagement under active (self-initiated) and passive (experimenter-initiated) conditions.

The primary objective of this analysis is to elucidate the underlying neural structures that differentiate active from passive engagement. By examining the synchronization of cell assemblies, the temporal alignment of neural activity with behavioral events, and the consistency of neural responses across trials, we aim to provide a comprehensive understanding of how neural coordination and adaptability are influenced by behavioral context. The results underscore the significance of active participation in enhancing neural efficiency, offering new perspectives on neural plasticity and cognitive function.

## Comprehensive Analysis of TCA Results

Tensor Component Analysis (TCA) is employed to decompose spike-train data recorded from the PVN into three modes: neurons, time, and trials. This method allows for the extraction of components that represent neuron-specific factors (neuron loading), temporal dynamics (time loading), and across-trial variability (trial loading). Unlike standard dimensionality reduction techniques, TCA leverages the multi-dimensional structure of the data to reveal patterns that are unique to each mode. This section delves into the analysis of these components, focusing on the differences observed between active and passive engagement conditions.

## Neuron Factors: Identifying Coherent Cell Assemblies

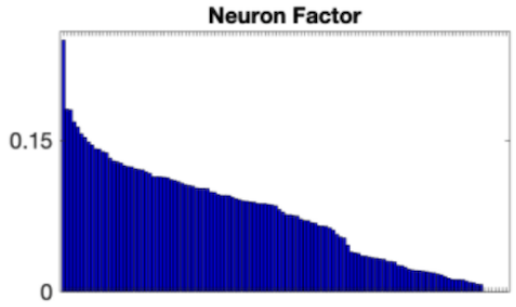


Figure 9: Neuron factors during active engagement. Neurons are more coherently clustered, indicating enhanced synchrony and coordination among cell assemblies.

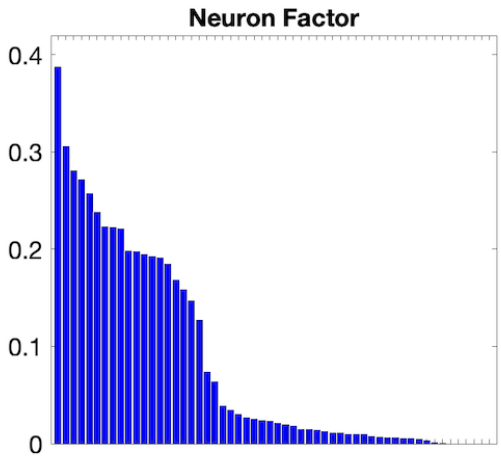


Figure 10: Neuron factors during passive engagement. The more diffuse distribution of neuron factors suggests less coordinated activity.

Figures 9 and 10 show the neuron factors derived from TCA for active and passive conditions, respectively. These neuron factors represent the contribution of each neuron to specific components, effectively highlighting the emergence of cell assemblies involved in coordinated activity.

Under active engagement, the neuron factors demonstrate a tighter clustering of neurons, indicating more coherent participation of specific neurons in task-relevant neural assemblies. This pattern suggests that active engagement leads to higher neural synchrony within these assemblies, potentially optimizing the network for encoding complex, behaviorally relevant information. The increased neural synchrony is consistent with the concept that active involvement enhances the brain's ability to allocate neural resources more effectively.

In contrast, the neuron factors in passive engagement conditions display a more scattered distribution, which implies a lack of robust coordination among neurons. This may reflect a reduced capacity for forming stable cell assemblies due to the absence of volitional engagement, leading to less efficient neural processing. This finding aligns with the hypothesis that passive engagement is less effective in driving adaptive neural changes.

## Temporal Dynamics: Capturing Within-Trial Neural Responses

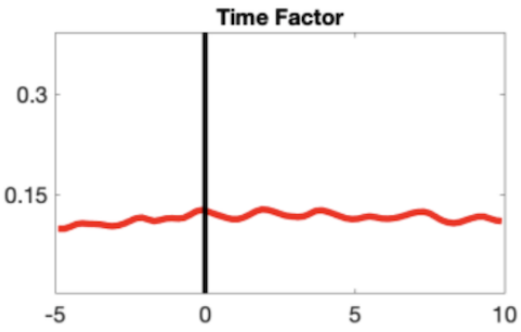


Figure 11: Temporal factors during active engagement. The sharp, well-defined peaks correspond to key behavioral events, reflecting precise and coordinated neural responses.

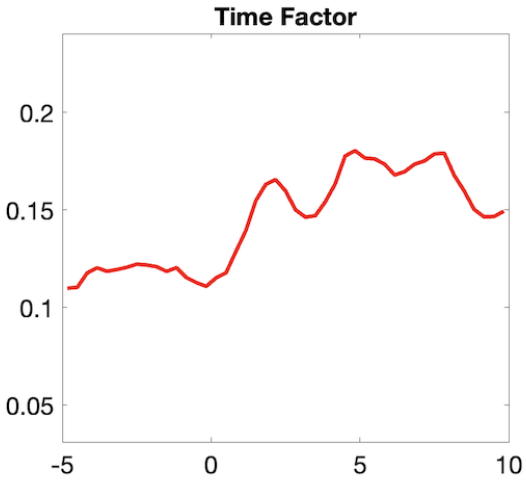


Figure 12: Temporal factors during passive engagement. Broader, less distinct peaks suggest weaker temporal synchronization of neural responses.

Figures 11 and 12 present the temporal factors extracted from TCA for both engagement conditions. Temporal factors provide insight into how neural activity fluctuates over time relative to stimulus onset or behavioral events. In the active condition, these factors reveal sharp, well-defined peaks that align closely with key moments, such as the onset of stimuli in behavioral tasks. This indicates a high level of temporal coordination in the neural response, suggesting that active engagement enhances the precision with which neural circuits respond to relevant stimuli.

Conversely, in the passive condition, the temporal factors exhibit broader, less distinct peaks, indicating a less synchronized neural response. This could suggest that when stimuli are not self-initiated, the neural circuits may not be as primed for precise, event-driven responses. The broader temporal dynamics reflect a more generalized response pattern that might underlie reduced neural efficiency in encoding stimulus-specific information.

### Trial Factors: Evaluating Across-Trial Consistency and Variability

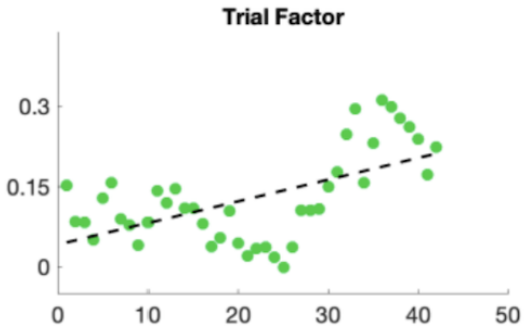


Figure 13: Trial factors during active engagement. The consistent patterns suggest stable engagement and efficient adaptation across trials.

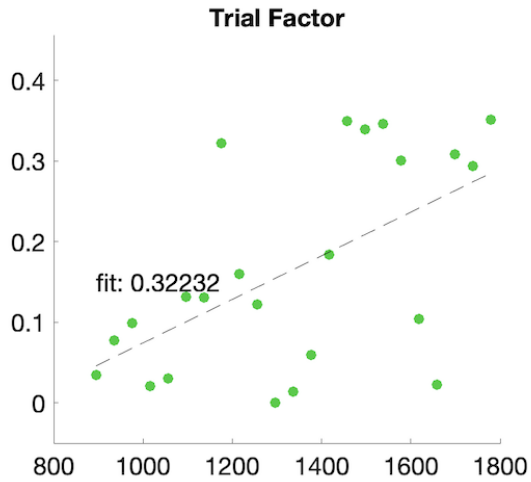


Figure 14: Trial factors during passive engagement. The significant variability indicates less stable neural engagement across trials.

Figures 13 and 14 illustrate the trial factors derived from the TCA, capturing the consistency and variability of neural responses across multiple trials. In the active engagement scenario, the trial components exhibit strong and consistent patterns, indicating that the neural circuits are robustly engaged and adapt effectively over repeated trials. This finding is indicative of stable synaptic changes and efficient neural plasticity, which is essential for learning and memory consolidation.

In contrast, the trial factors for passive conditions show significant variability, suggesting less effective neural adaptation. This variability may reflect a lack of consistent engagement of neural circuits in response to externally initiated stimuli, which could hinder the development of stable neural representations necessary for long-term learning and adaptation.

## Conclusion

This chapter presents an advanced analysis of neural dynamics using Tensor Component Analysis (TCA) to understand the differences between active and passive engagement in behavioral paradigms. By decomposing high-dimensional neural data

into neuron, temporal, and trial components, the study reveals that active engagement conditions are associated with more distinct, coherent, and synchronized patterns of neural activity.

The Neuron Factors highlight the formation of coordinated cell assemblies under active conditions, suggesting that volitional engagement enhances neural synchrony and resource allocation. The Time Factors provide insights into the temporal alignment of neural activity with behavioral events, where active engagement shows sharper, more pronounced peaks that indicate precise temporal coordination. Trial Factors reveal the consistency and variability of neural engagement across multiple trials, with active conditions demonstrating strong, stable patterns aligned with efficient learning and adaptation.

Overall, this analysis underscores the importance of active engagement in driving more efficient neural processing and adaptation. The results suggest new avenues for future research, such as exploring the impact of engagement-driven neural dynamics across different brain regions, using additional connectivity measures, and examining how these dynamics can be leveraged for cognitive enhancement strategies or neural rehabilitation.

# Discussion

The present study investigates the neural mechanisms underlying the acquisition and expression of maternal behavior in mice, specifically focusing on the role of the hypothalamic paraventricular nucleus (PVN) and the neuropeptide oxytocin. By employing Tensor Component Analysis (TCA) to analyze complex, high-dimensional neural data, this research elucidates the neural dynamics associated with different levels of engagement in maternal behavior learning. The findings are discussed in the context of existing literature, highlighting both the advancements made in understanding the neural basis of maternal behavior and the implications for computational neuroscience.

## Neural Mechanisms Underlying Maternal Behavior Learning

The results of this study provide compelling evidence that neural plasticity within the PVN plays a crucial role in the learning and expression of maternal behaviors, particularly in non-biological parenting scenarios. The use of TCA enabled the decomposition of neural activity into interpretable components, revealing distinct neural patterns associated with varying levels of engagement in the learning process. Specifically, the findings indicate that active engagement in learning—where mice are allowed to exercise volitional control over the observation of maternal behaviors—results in more coherent and synchronized neural activity compared to passive engagement, where learning is imposed without volition.

This aligns with previous research suggesting that oxytocinergic signaling within the PVN is crucial for facilitating social learning and bonding behaviors (Marlin et al., 2015; Burkett et al., 2016). The current study extends this understanding by demonstrating that oxytocin not only modulates social behaviors but also influences the plasticity of neural circuits in a manner that is engagement-dependent. This is particularly significant given that traditional models of maternal behavior have predominantly focused on biological parenting, whereas this study highlights the neural basis of alloparenting—a scenario more reflective of social learning processes.

## The Role of Active Versus Passive Engagement in Neural Learning Dynamics

The differentiation between active and passive engagement in learning maternal behavior provides novel insights into how behavioral states modulate neural dynamics.

The data indicate that active engagement, characterized by voluntary initiation of social learning stimuli, leads to more robust and synchronized neural activity within the PVN. This is evident from the sharper, well-defined peaks in the temporal components derived from TCA, as well as the more coherent clustering of neuron factors. Such findings are consistent with the hypothesis that active engagement enhances neural synchrony and resource allocation, optimizing the network for encoding complex, behaviorally relevant information (Engel et al., 2017).

In contrast, passive engagement results in broader, less distinct temporal components and a more diffuse distribution of neuron factors. This suggests a lack of robust coordination among neurons, potentially reflecting a reduced capacity for forming stable cell assemblies. These results align with studies in cognitive neuroscience that have shown that active participation in learning processes enhances synaptic plasticity and improves learning outcomes (Hampson et al., 2012; Dudai et al., 2015). The current study adds to this body of knowledge by demonstrating that similar principles apply to social learning contexts, particularly in the acquisition of complex social behaviors like maternal care.

## Implications for Computational Neuroscience and Machine Learning

The successful application of Tensor Component Analysis (TCA) to high-dimensional neural data represents a significant advancement in computational neuroscience. Traditional dimensionality reduction techniques, such as Principal Component Analysis (PCA) and Independent Component Analysis (ICA), have limitations in capturing the multi-dimensional and interactive nature of neural activity. TCA, by contrast, preserves the tensor structure of the data, allowing for a more nuanced decomposition that captures the interactions between neurons, time, and experimental conditions. This study's use of TCA not only provides a clearer picture of the neural dynamics underlying maternal behavior learning but also demonstrates the utility of advanced computational tools in neuroscience research.

Furthermore, the findings underscore the potential of integrating TCA with machine learning approaches to predict neural responses based on past activity. This opens up new avenues for developing models that can simulate complex neural dynamics and potentially inform the design of artificial neural networks (ANNs) that mimic biological processes. Future research could explore the integration of TCA with recurrent neural network (RNN) architectures to better understand how dynamic changes

in neural activity relate to specific behavioral outcomes.

## Gaps and Future Directions

While the study provides significant insights into the neural mechanisms underlying maternal behavior learning, several gaps remain that warrant further investigation. First, while the focus on the PVN and oxytocinergic signaling provides a targeted understanding of the neural basis of maternal behavior, the broader neural circuits involved in this process remain underexplored. Future studies could extend the analysis to other brain regions implicated in social behaviors, such as the medial preoptic area (MPOA) and the nucleus accumbens, to develop a more comprehensive model of the neural dynamics involved.

Second, the study's experimental design primarily relies on invasive recording techniques, which, while providing high-resolution data, may not fully capture the neural dynamics in more naturalistic settings. Future research could benefit from integrating non-invasive imaging techniques, such as functional magnetic resonance imaging (fMRI) or optogenetics, to complement the invasive methods used here and provide a more holistic view of the neural mechanisms at play.

Lastly, while the differentiation between active and passive engagement in learning provides valuable insights, the specific mechanisms by which oxytocin modulates neural plasticity in these different contexts remain to be fully elucidated. Further studies could employ pharmacological manipulations to selectively modulate oxytocin receptors and investigate how such interventions affect both the neural and behavioral outcomes of social learning.

# 5. Conclusion

This study makes a substantial contribution to our understanding of the neural mechanisms underlying maternal behavior, particularly in the context of social learning and alloparenting. By leveraging advanced computational tools like Tensor Component Analysis (TCA), the research reveals distinct neural dynamics associated with different levels of engagement in maternal behavior learning, highlighting the importance of active participation in enhancing neural synchrony and efficiency. The findings have broad implications for computational neuroscience, providing a robust framework for future studies aimed at dissecting complex neural dynamics. Future research should focus on expanding the scope of neural recordings to other relevant brain regions, integrating non-invasive techniques, and further elucidating the role

of neuropeptides like oxytocin in modulating neural plasticity in socially relevant contexts.

# Conclusion

This thesis has explored the neural mechanisms underlying the learning and expression of maternal behaviors in mice, focusing on the hypothalamic paraventricular nucleus (PVN) and its modulation by oxytocin. By employing Tensor Component Analysis (TCA) on high-dimensional neural data, the research has uncovered distinct neural patterns associated with different levels of engagement in maternal behavior learning. This study not only advances our understanding of the PVN's role in social learning but also provides a robust computational framework for analyzing complex neural dynamics. The findings have broad implications for neuroscience, machine learning, and our understanding of the neurobiological basis of social behavior.

## Summary of Key Findings

This research has provided significant insights into the neural basis of maternal behavior learning through several key findings. First, it successfully modeled the global neural activity within the PVN during different stages of maternal behavior learning, revealing specific patterns of neural activation critical for both the learning and expression of these behaviors. The study highlighted the role of oxytocinergic signaling in facilitating these behaviors, suggesting that the PVN's neural circuits undergo significant reorganization in response to socially relevant cues.

Second, the application of Tensor Component Analysis (TCA) was demonstrated to be highly effective for analyzing high-dimensional neural data. Unlike traditional methods such as PCA or ICA, TCA preserved the multi-dimensional structure of the data, allowing for a more comprehensive understanding of the interactions between neurons, time, and behavioral conditions. This enabled the identification of distinct neural components associated with varying levels of engagement in learning maternal behaviors, providing deeper insights into the neural underpinnings of social learning.

Finally, the study differentiated between active and passive engagement in maternal behavior learning, showing that active engagement leads to more synchronized and coherent neural activity. This suggests that volitional control enhances the brain's ability to allocate neural resources more effectively, optimizing learning and memory processes. Additionally, the exploration of effective connectivity between PVN neurons revealed how specific neural circuits are dynamically modulated in response to social stimuli, providing a foundation for future studies aimed at mapping the complete network of brain regions involved in maternal behavior and social

learning.

## Implications for Neuroscience and Machine Learning

The findings of this thesis have significant implications for both neuroscience and computational methodologies. From a neuroscience perspective, this research contributes to a more nuanced understanding of the neural mechanisms underlying social behaviors, particularly maternal behaviors. The focus on the PVN and its modulation by oxytocin offers new insights into the neurobiological basis of social learning, highlighting the importance of engagement-dependent neural plasticity. These findings open up new avenues for exploring how other neuropeptides and brain regions interact to shape complex social behaviors, such as caregiving, bonding, and empathy.

From a computational neuroscience and machine learning standpoint, the successful application of TCA demonstrates the potential of advanced computational tools to uncover complex neural dynamics. The ability of TCA to handle high-dimensional data and extract meaningful patterns sets a precedent for its use in other areas of neuroscience. Moreover, integrating TCA with machine learning approaches, such as recurrent neural networks (RNNs), could lead to more sophisticated models that simulate neural activity and predict behavioral outcomes. This integration could inform the design of artificial neural networks (ANNs) that better mimic biological processes, potentially advancing the field of artificial intelligence.

## Limitations and Future Directions

While this study provides significant advancements, several limitations must be acknowledged, which also pave the way for future research. One limitation is the scope of neural recording, which primarily focused on the PVN. While this focus provides a targeted understanding of oxytocin's role in social behavior, maternal behavior is a complex process involving various brain regions, including the medial preoptic area (MPOA), the nucleus accumbens, and the amygdala. Future research should extend the neural recording scope to these regions to develop a more comprehensive model of the brain circuits involved in social learning and maternal behavior.

Additionally, while the use of invasive recording techniques allowed for high-resolution data collection, it may not fully capture the neural dynamics that occur in more naturalistic settings. Future studies could incorporate non-invasive imaging methods, such as fMRI or calcium imaging, to validate the findings under conditions that better mimic natural environments. This would help bridge the gap between

highly controlled experimental setups and real-world applications.

Another limitation is that, although the study demonstrated that oxytocin plays a crucial role in modulating neural plasticity, the specific mechanisms by which oxytocin influences neural circuits in different engagement contexts remain to be fully elucidated. Further research involving targeted pharmacological manipulations and genetic approaches could provide more precise insights into the cellular and molecular mechanisms of oxytocin's effects on social learning.

Finally, while the use of TCA has proven effective, future research could explore integrating TCA with other computational techniques, such as supervised learning models or reinforcement learning frameworks. This integration could help better link neural activity patterns to behavioral outputs and provide more comprehensive models of brain function.

## Concluding Remarks

This thesis has made significant contributions to understanding the neural dynamics of maternal behavior learning and the role of engagement-dependent plasticity. By combining advanced computational methods with rigorous experimental techniques, this research bridges the gap between theoretical models and empirical data, offering valuable insights into the complex interplay between neural activity, social learning, and behavior. As neuroscience continues to evolve, the methodologies and findings presented in this work will serve as a foundation for future studies aimed at unraveling the neural mechanisms underlying complex social behaviors, ultimately contributing to the broader fields of computational neuroscience, artificial intelligence, and behavioral research.

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# Appendices

## 0.1 Theoretical and Computational Methods

### 0.1.1 Tensor Component Analysis (TCA) Derivation

**Objective**: Minimize the reconstruction error in the tensor decomposition.

**Mathematical Formulation**:

$$\min_{\mathbf{A},\mathbf{B},\mathbf{C}} \left\| \mathcal{X} - \sum_{r=1}^{R} \lambda_r \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r \right\|_F^2 \tag{1}$$

where $\mathcal{X} \in \mathbb{R}^{N \times T \times K}$ is the tensor, and $\mathbf{A} \in \mathbb{R}^{N \times R}$, $\mathbf{B} \in \mathbb{R}^{T \times R}$, $\mathbf{C} \in \mathbb{R}^{K \times R}$ are the factor matrices.

**Derivation Steps**:

1. **Unfolding the Tensor**: The tensor is unfolded into matrices corresponding to each mode (e.g., mode-1 unfolding). Unfolding uses Kronecker and Khatri-Rao products to transform the tensor into matrix forms suitable for optimization.

2. **Alternating Least Squares (ALS)**: ALS is used to iteratively update the factor matrices by solving least squares problems for each mode. The Khatri-Rao product efficiently computes updates for the factor matrices.

3. **Optimization**: The optimization problem involves minimizing the Frobenius norm between the original tensor $\mathcal{X}$ and its low-rank approximation. The solution is typically non-convex, and ALS is employed to solve for $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ iteratively to minimize the reconstruction error.

4. **Role of Regularization**: Regularization techniques, such as L2 norm regularization, are introduced to control overfitting by adding penalty terms that limit the magnitude of the factor matrices.

**Additional Details on Computational Efficiency**:

- The Kronecker and Khatri-Rao products play a pivotal role in the computational steps of TCA, particularly in the optimization process. For example, the Kronecker product expands matrices, facilitating tensor unfolding, while the Khatri-Rao product simplifies combining factor matrices during updates.

- Tensor decompositions such as Tucker and CP (CANDECOMP/PARAFAC) are also essential methods. Tucker decomposition generalizes PCA by decomposing a tensor into a core tensor and factor matrices, while CP simplifies to a sum of rank-one tensors when the core tensor is diagonal.

### 0.1.2 Transfer Entropy (TE) Calculation

**Objective**: Quantify the information flow between neurons.

**Mathematical Formulation**:

$$TE_{X\to Y} = \sum_{x_t, y_{t+1}, y_t} p(y_{t+1}, y_t, x_t) \log \frac{p(y_{t+1}|y_t, x_t)}{p(y_{t+1}|y_t)} \tag{2}$$

where $X_t$ and $Y_t$ are time series representing neuronal activities.

**Derivation Steps**:

1. **Joint Probability Estimation**: Methods such as kernel density estimation (KDE), generalized linear models (GLM), or autoregressive (AR) models are employed to estimate the required joint and conditional probabilities.

2. **Calculation**: Substituting these estimates into the TE formula allows for the computation of the directional information flow between neurons.

3. **Visualization**: Directed graphs or matrices are utilized to visualize the TE results, where nodes represent neurons and edges denote the direction and strength of information transfer.

### 0.1.3 Extended Experimental Protocols

**Freely Moving Learning Experiments**

**Setup and Conditions**:

- Detailed descriptions of the apparatus, including dimensions, materials, and specific configurations for each experimental condition (e.g., direct interaction, transparent barrier, opaque barrier). Calibration procedures are included to ensure consistency across experiments.

**Animal Handling**:

- Protocols for handling and preparing the animals are designed to ensure minimal stress and consistent conditions. These protocols emphasize standardized handling techniques to avoid introducing variability.

**Behavioral Measurements**:

- Detailed descriptions of the criteria used to measure maternal behaviors, including specific behaviors observed and how they were quantified. Metrics such as latency to retrieve pups and time spent grooming are recorded.

**Screen-Based Learning Experiments**

**Video Stimulus Design**:

- Specifications for the retrieval video, including duration, frame rate, and content, along with the rationale for selecting these parameters. The videos replicate naturalistic pup-retrieval scenarios to maximize ecological validity.

**Presentation Protocol**:

- Setup for presenting video stimuli to animals, including screen type, distance from animals, and ambient conditions. Control for extraneous variables such as ambient light and sound is critical to maintaining a controlled experimental environment.

### 0.1.4 Neural Recording Procedures

**Buzsaki32L Probe Details**:

- Specifications for the Buzsaki32L probe, including exact placement within the PVN, implantation procedure, and calibration of the recording equipment. The probe's high-density design allows for comprehensive recordings of single-unit and multi-unit activity.

**Data Acquisition**:

- Procedures for neural data acquisition include sampling rates, filtering techniques, and the duration of recordings for each experimental condition. The use of advanced spike-sorting algorithms (e.g., Kilosort2) and machine learning methods ensures accurate detection of neuronal firing patterns.

**Spike Sorting and Feature Extraction**:

- Spike sorting is performed using Kilosort2, followed by manual curation with Phy. Clusters are validated using isolation distance, L-ratio, and refractory period violations to ensure that recorded spikes represent well-isolated single units.

**Dimensionality Reduction and Component Clustering**:

- Tensor Component Analysis (TCA) is applied to identify low-dimensional representations of neural activity. Subsequent clustering of TCA components identifies functionally relevant groups and assesses component stability across sessions.

## 0.2 Supplementary Mathematical Details

### 0.2.1 Kronecker and Khatri-Rao Products

**Kronecker Product**:

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{pmatrix} \tag{3}$$

**Khatri-Rao Product**:

$$\mathbf{A} \odot \mathbf{B} = [a_1 \otimes b_1 \, a_2 \otimes b_2 \, \cdots \, a_r \otimes b_r] \tag{4}$$

These products are essential for tensor unfolding and efficient computation in the optimization process of TCA.

### 0.2.2 Mode-n Products and Tensor Unfolding

**Mode-n Product Definition**:

$$(\mathcal{X} \times_n \mathbf{A})_{i_1,\ldots,i_{n-1},j,i_{n+1},\ldots,i_N} = \sum_{i_n} x_{i_1,i_2,\ldots,i_N} a_{j,i_n} \tag{5}$$

**Tensor Unfolding Examples**:

- **Mode-1 unfolding:** $X(1)$ of size $N \times (T \times K)$
- **Mode-2 unfolding:** $X(2)$ of size $T \times (N \times K)$

- **Mode-3 unfolding:** $X(3)$ of size $K \times (N \times T)$

These operations are integral to implementing TCA, enabling the transformation of tensors into matrices that facilitate the ALS optimization algorithm.