Deep Exponential-Family Auto-Encoders

Bahareh Tolooshams\textsuperscript{1}, Andrew H. Song\textsuperscript{2}, Simona Temereanca\textsuperscript{3}, and Demba Ba\textsuperscript{1}

\textsuperscript{1}Harvard University  \\
\textsuperscript{2}Massachusetts Institute of Technology  \\
\textsuperscript{3}Brown University

Abstract

We consider the problem of learning recurring convolutional patterns from data that are not necessarily real valued, such as binary or count-valued data. We cast the problem as one of learning a convolutional dictionary, subject to sparsity constraints, given observations drawn from a distribution that belongs to the canonical exponential family. We propose two general approaches towards its solution. The first approach uses the \(\ell_0\) pseudo-norm to enforce sparsity and is reminiscent of the alternating-minimization algorithm for classical convolutional dictionary learning (CDL). The second approach, which uses the \(\ell_1\) norm to enforce sparsity, generalizes to the exponential family the recently-shown connection between CDL and a class of ReLU auto-encoders for Gaussian observations. The two approaches can each be interpreted as an auto-encoder, the weights of which are in one-to-one correspondence with the parameters of the convolutional dictionary. Our key insight is that, unless the observations are Gaussian valued, the input fed into the encoder ought to be modified iteratively, and in a specific manner, using the parameters of the dictionary. Compared to the \(\ell_0\) approach, once trained, the forward pass through the \(\ell_1\) encoder computes sparse codes orders of magnitude more efficiently. We apply the two approaches to the unsupervised learning of the stimulus effect from neural spiking data acquired in the barrel cortex of mice in response to periodic whisker deflections. We demonstrate that they are both superior to generalized linear models, which rely on hand-crafted features.

1 Introduction

In the signal processing literature, convolutional dictionary learning (CDL) is the de-facto method for learning sparse signal representations that are tailored to a given dataset [1]. In machine learning, deep learning has become a popular method for learning signal representations from data [2]. CDL algorithms and deep convolutional neural networks (NNs) learn local patterns that are common to the examples comprising the dataset of interest.

CDL assumes that every example \(y\) from the dataset admits a representation as a sparse linear combination of locally shifted filters. Mathematically, in the absence of noise, we can express this as \(y = Hx\), where \(H\) is a convolutional matrix comprising locally shifted copies of the filters, and \(x\) is a sparse code vector whose nonzero elements select where each of the filters occurs in \(y\). The goal of classical CDL is to learn \(H\) and \(x\) using all examples [1]. Classical methods cast this as a non-convex optimization problem. To deal with the non convexity, most CDL frameworks [1] proceed by alternating minimization, iterating between a convolutional sparse coding step and a dictionary update step. When the data \(y\) are real valued, a recent line of work [3, 4, 5] has shown a one-to-one correspondence between classical optimization-based CDL algorithms and a class of deep ReLU networks. The advantage to this correspondence is two-fold. First, it provides a principled framework for solving CDL problems using NNs. Second, it makes it possible to solve CDL problems using GPUs, orders of magnitude faster than optimization-based algorithms for CDL. While classical CDL has been successful in a number of applications [1, 4], the majority of existing work assumes that the data of interest are real valued and are therefore not appropriate for data that are binary or count valued such as neural spiking data, fingerprint images, and photon-based images, to name a few. There have been several attempts to address this in the context of sparse coding [6, 7], and more recently dictionary learning for count data contaminated by Poisson noise [8, 9]. These analyses, however, assume patch-based, as opposed to convolutional, representations of the data of interest and rely on restrictive assumptions on the data generating process. The dearth of principled approaches for learning convolutional representations from data that are not real valued is even more pronounced in the deep learning field. To our knowledge, there does not exist a rigorous framework for training deep NNs using such data. Restricted Boltzmann machines (RBMs) [10] can accommodate binary data. However, RBMs assume the hidden features underlying the input data are binary.

We propose two general frameworks for learning convolutional representations, subject to sparsity constraints, from data drawn from a distribution in the canonical exponential family. Both algorithms draw inspiration from the iteratively reweighted least squares (IRLS) algorithm [11] for maximum likelihood estimation in the canonical exponential family. The first framework, termed exponential-family convolutional orthogonal matching pursuit (ECOMP), uses the \(\ell_0\) pseudo-norm to enforce sparsity. ECOMP is an alternating-minimization algorithm for optimization-based CDL. The sparse coding step extends OMP [12] to the exponential family. The dictionary update step is a constrained maximum likelihood estimation problem using the distribution of interest. The second framework,
which uses the $L_1$ norm to enforce sparsity, is inspired by the recent connections developed in the signal processing literature between alternating-minimization algorithms and deep constrained auto-encoders [3]. Our approach maps the alternating-minimization algorithm for $L_1$-based CDL to a constrained deep neural network which we call deep exponential-family auto-encoder (DEA). The encoder performs ISTA [13] on iteratively modified versions of the input data and outputs sparse codes. The decoder uses the output of the encoder to construct the likelihood of the exponential family of interest. Fig. 1 demonstrates the general architecture for the two proposed frameworks.

**Figure 1**: Generic auto-encoder architecture for canonical exponential-family convolutional dictionary learning. The encoder/decoder structure mimics the sparse coding and dictionary update steps in optimization-based alternating-minimization algorithms for dictionary learning. The black box corresponds to either $L_0$-based (ECOMP) or $L_1$-based (DEA) sparse coding. The encoder performs $T$ iterations of sparse coding. Each iteration uses “working observations” $\tilde{y}$, obtained by iteratively modifying the inputs $y$ using the filters $H$ and a nonlinearity $f(\cdot)^{-1}$ that depends on the specific distribution in the canonical exponential family that the observations $y$ are drawn from. To update the dictionary, the decoder applies a loss, which also depends on the distribution of the observations, to a linear function of the output $x_T$ of the encoder.

Our main contributions are as follows

**NNs for non-real-valued data** We propose a general principled prescription, not only for learning a convolutional dictionary using exponential family data, but also for designing and training NNs using such data.

**Fast inference in NNs for non-real-valued data** We show through simulation that the encoders of ECOMP and DEA perform inference faster than CVXPY [14], a popular convex optimization library, respectively by factors of 4x and 70x. The superiority of the DEA encoder comes from the fact that it can be easily deployed on GPUs.

**Unsupervised learning of stimulus effect in models of neural spiking data** We apply ECOMP and DEA to the unsupervised learning of the stimulus effect in simulated and real neural spiking data from neurons in the barrel cortex. Our results demonstrate that ECOMP and DEA can be applied to a linear function of the output $x_T$ of the encoder.

## 2 Problem Formulation

### Canonical exponential-family distribution

For a given observation vector $y \in \mathbb{R}^N$, with mean $\mu \in \mathbb{R}^N$, we define the log-likelihood of the canonical exponential family [16] as

$$
\log p(y|\mu) = f(\mu)^T y + g(y) - B(\mu),
$$

where we have assumed that, conditioned on $\mu$, the elements of $y$ are independent. The canonical exponential family includes a broad family of probability distributions such as the Normal, Bernoulli, Poisson, and Gamma distributions. The functions $g(\cdot)$, $B(\cdot)$, as well as the invertible link function $f(\cdot)$, all depend on the choice of distribution. Let $A \in \mathbb{R}^{N \times p}$ denote a generic design matrix whose columns correspond to covariates and $x \in \mathbb{R}^p$ a vector of coefficients. If we let $f(\mu) = Ax$, or equivalently $\mu = f^{-1}(Ax)$, then Eq. 1 becomes a GLM [16] with canonical link $f(\cdot)$. Given $y$, maximizing the log-likelihood using Newton’s method leads to an IRLS algorithm. In IRLS, each Newton iteration corresponds to covariates and $\mu$. Each iteration uses “working observations” $\tilde{y}$, obtained by iteratively modifying the inputs $y$ using the filters $H$ and a nonlinearity $f(\cdot)^{-1}$ that depends on the specific distribution in the canonical exponential family that the observations $y$ are drawn from. To update the dictionary, the decoder applies a loss, which also depends on the distribution of the observations, to a linear function of the output $x_T$ of the encoder.

$$
\nabla_\mu \log p(y|\mu) = \nabla_\mu \log p(y|A, x) = A^T (y - f^{-1}(Ax)),
$$

which represents the inner product between the columns of $A$ and the working observation $\tilde{y}$.

**Convolutedal GLM** We consider the setting in which the linear predictor is the sum of scaled and time-shifted copies of $C$ finite-length filters, denoted $\{h_c\}_{c=1}^C \in \mathbb{R}^N$, each localized in time, i.e. $K < N$. Following notation and terminology from the signal processing literature [1], we can express $f(\mu)$ in convolutional form: $f(\mu) = \sum_{c=1}^C h_c * x^c$, where $*$ is the convolution operation, and $x^c \in \mathbb{R}^{N-K+1}$ is a train of scaled impulses which we refer to as code vector. We can use linear-algebraic notation to write $f(\mu) = \sum_{c=1}^C h_c * x^c = Hx$, where $H \in \mathbb{R}^{N \times (N-K+1)}$ is a matrix that is the concatenation of $C$ Toeplitz matrices $H_c \in \mathbb{R}^{N \times (N-K+1)}$, $c = 1, \ldots, C$, and $x = \{x^1, \ldots, x^C\}^T \in \mathbb{R}^{C(N-K+1)}$ is a vector with $C$ blocks, each of which is in one-to-one correspondence with the blocks of $H$. The columns...
of \( H \) consist of all possible time shifts of \( h_c \), zero-padded to have length \( N \). In the convolutional setting, we interpret \( y \) as a time series in discrete-time, and the non-zero elements of \( x \) as the times when each of the \( C \) filters contributes to the mean \( \mu \) of \( y \).

### 3 Methods

Given \( J \) observations \( \{y^j\}_{j=1}^J \), our goal is to estimate \( \{h_c\}_{c=1}^C \) and \( \{x^j\}_{j=1}^J \) that minimize the negative log likelihood \( -\sum_{j=1}^J \log p(y^j|\{h_c\}_{c=1}^C, x^j) \) under the canonical exponential family convolutional generative model, subject to sparsity constraints on the \( J \) code vectors \( \{x^j\}_{j=1}^J \). We enforce sparsity using either the \( \ell_0 \) pseudo-norm or the \( \ell_1 \) norm. This leads to the exponential-family convolutional dictionary learning (ECDL) problem

\[
\min \left\{ \sum_{j=1}^J \left( - (H x)^T y^j + B(f^{-1}(H x)) \right), \text{s.t. } x^j \geq 0, \|h_c\|_2 = 1, \left\{ \begin{array}{l} \|x^j\|_0 \leq \beta_0 \\
\|x^j\|_1 \leq \beta_1 \end{array} \right. \right\} \quad (3)
\]

where \( \beta_0 \) and \( \beta_1 \) are hyperparameters that control the degree of sparsity. The non-negativity constraint is a natural choice in applications of both CDL [1] and deep NNs [17]. The objective is jointly non convex in \( H \) and \( x^j \). A popular approach to deal with the non convexity is to alternatively minimize the objective over one set of variables while the others are fixed, until convergence. Let \( m \geq 1 \) denote the \( m \)th iteration of the alternating-minimization procedure. At iteration \( m+1 \), the codes \( \{x^j\}_{j=1}^J \) are computed based on \( H^{(m)} \) through a convolutional sparse coding step, after which \( H^{(m+1)} \) is computed using \( \{x^j\}_{j=1}^J \) through a convolutional dictionary update step.

Motivated by the alternating-minimization algorithm described above, we present two approaches to solve the ECDL problem: 1) ECOMP and 2) a DEA architecture. ECOMP uses the \( \ell_0 \) pseudo-norm to enforce sparsity and generalizes to the exponential family classical optimization-based algorithms for \( \ell_0 \)-based CDL. DEAs use the \( \ell_1 \) norm to enforce sparsity and generalize the convolutional recurrent sparse auto-encoders from [5] to the exponential family. To simplify the notation, we drop the superscript \( m \) in the rest of this section.

#### 3.1 Alternating-minimization Algorithm for Greedy ECDL

\( \ell_0 \)-based convolutional sparse coding in the canonical exponential family. Eq. 3 with the \( \ell_0 \) constraint is a combinatorially-hard optimization problem. We use a greedy approach that is an extension of OMP [12], which was originally designed for real-valued observations. To simplify the notation further, we drop the superscript \( m \).

Because of the convolutional structure of dictionary, we can accelerate the selection step by replacing the multiplication with \( H^T \) by \( C \) cross-correlation operations as follows

\[
H^T \tilde{y}_i = [\langle h_1, \tilde{y}_i \rangle [0], \ldots, \langle h_1, \tilde{y}_i \rangle [N-K], \ldots, \langle h_C, \tilde{y}_i \rangle [0], \ldots, \langle h_C, \tilde{y}_i \rangle [N-K]]^T \quad (4)
\]

where \( \bullet \) denotes the cross-correlation operation. This approach is computationally efficient as only \( C \) cross-correlation operations are required, compared to \( C(K - N + 1) \) multiplications. It is also memory efficient as we do not need to construct the convolutional dictionary \( H \) explicitly to compute the cross-correlations.

Convolutional dictionary update in the canonical exponential family. To update the convolutional dictionary, we use the commutativity of the convolution operation to switch the roles of \( H \) and \( x \). We treat \( x \) as the filter and construct the Toeplitz matrix \( X \) such that

\[
H X = \sum_{c=1}^C \sum_{i=1}^{N-K} X_{c,i} h_c
\]
where \( N_i = |x_i| \), \( X_{c,i} = \left[ 0_{N_c \times K} \right] x^T \left[ 0_{N_c - 1} \cdot 0_{N_c - 1} \right] \in \mathbb{R}^{N \times K} \), and \( n_{c,i} \) is the time of occurrence of the \( i \)th event from filter \( c \) (nonzero entry of \( x^T \)).

We are now in a position to optimize the negative log-likelihood with respect to \( \{ h_c \}_{c=1}^C \). The objective is a constrained convex optimization problem, which can be solved with the standard techniques mentioned above for the sparse coding step. We fill in some details pertaining to ECOMP in Algorithm 1 of the Supplementary Material section.

**Figure 2:** Black box associated with the ECOMP architecture. The black box performs sparse coding by greedy pursuit. We can interpret the selection step as performing max pooling, with memory of the location of the max, on the correlation between \( \tilde{y}_t \) and the filters. This is followed by the linear projection step.

**Connection to encoder architecture** Conceptually, we can map a single iteration of the alternating-minimization algorithm for ECDL by ECOMP to the encoder diagram depicted in Fig. 1, and further illustrated in Fig. 2. The encoder first computes the working observation \( \tilde{y}_t \) from a given input \( y \). The working observation then goes through the cascade of a 1) multiplication with \( H^T \), equivalent to computing an inner product or cross-correlation, 2) max pooling with memory of the location of the max, equivalent to greedy selection of a filter, and 3) a projection step. In the next section, we develop this encoder analogy further in the case when one imposes sparsity in Eq. 3 using the \( \ell_1 \) norm.

### 3.2 Deep Exponential-Family Auto-Encoders for ECDL

**\( \ell_1 \)-based exponential-family auto-encoders** We generalize the deep residual auto-encoder introduced in [3, 4], for learning a convolutional dictionary from real valued data, to data drawn from a distribution in the exponential family. We name this generalization deep exponential-family auto-encoder (DEA). The overall structure of the encoder parallels the convolutional sparse coding step in the optimization-based alternating-minimization scheme. The decoder, together with a loss function derived from the log-likelihood, parallels the dictionary update step. In the training stage, we update the filters by backpropagation through the auto-encoder.

**Encoder** The forward pass of the encoder maps inputs \( y^j \) into sparse codes \( x^j \). To simplify the notation, we drop the superscript \( j \). Given filters \( \{ h_c \}_{c=1}^C \), the encoder solves the following unconstrained version of the \( \ell_1 \)-regularized optimization problem from Eq. 3

\[
\min_{x \geq 0} \ - \log p(y | \{ h_c \}_{c=1}^C, x) + \lambda \|x\|_1
\]

using \( T \) iterations of ISTA [13]. One iteration of ISTA is given by

\[
x_t = \text{ReLU} \left( \frac{1}{L} H^T (y - f^{-1}(Hx_{t-1})) - \frac{\lambda}{L} \right) = \text{ReLU} \left( x_{t-1} + \frac{1}{L} H^T \tilde{y}_t - \frac{\lambda}{L} \right) \quad \text{(6)}
\]

where \( x_t \) denotes the sparse code after \( t \) iterations of ISTA, and \( \frac{1}{L} \) is the step size of the gradient update of the code. The architecture of the encoder is a recurrent one that arises by unfolding \( T \) iterations of ISTA and is reminiscent of deep unfolding [19]. Fig. 3 depicts the recurrent encoder. It corresponds to the black box from Fig. 1 that is associated with the DEA architecture. In Fig. 1, \( f^{-1}(\cdot) \) is the inverse of the link function associated with the observations. We can also interpret it as a nonlinear activation function. For Gaussian observations, \( f^{-1}(\cdot) \) is linear with slope 1. However, for data drawn from a distribution from the canonical exponential family, the encoder uses \( f^{-1}(\cdot) \) to transform the input \( y \) at each iteration into a continuous-valued working observation \( \tilde{y}_t \). The matrix \( H^T \) performs pattern recognition by computing the correlation of the working observation with the filters. The output of the correlation goes through a ReLU nonlinearity to obtain a sparse embedding of the input \( y \). The ReLU arises from the \( \ell_1 \) norm and the non-negativity constraint in Eq. 5 on the elements of \( x \).

**Decoder** We apply a linear decoder \( H \) to the output of the encoder \( x_T \) to obtain the linear predictor \( Hx_T \). This decoder completes the forward pass of the DEA architecture. Algorithm 2 from the

\[
\frac{1}{L} H^T \tilde{y}_t - \frac{\lambda}{L} \quad \text{(6)}
\]
The objective is to learn from the data the features of whisker motion that modulate neural spiking.

Training the DEA architecture

The overall architecture uses linear operators $H$ for convolution and $H^T$ for correlation. Both are fully determined by the filters $\{h_c\}_{c=1}^C$, which are the parameters, i.e., weights, of interest. We train the weights by backpropagation through the auto-encoder using the loss function from Eq. 7.

\[
\mathcal{L}_H(\mathbf{y}, \{h_c\}_{c=1}^C, \lambda, L) = -\log p(\mathbf{y} \mid \{h_c\}_{c=1}^C, \mathbf{x}_T)
\]  

(7)

4 Applications to Neural Spiking Data from Barrel Cortex

Classical GLM analyses do not capture experimental non idealities

We apply ECDL to simulated and real data from barrel cortex recorded in response to periodic whisker deflections [20]. The objective is to learn from the data the features of whisker motion that modulate neural spiking strongly.

Previous analyses using GLMs reported that the neurons from this experiment encode strongly. Previous analyses using GLMs reported that the neurons from this experiment encode

\[
\mathcal{L}_H(\mathbf{y}, \{h_c\}_{c=1}^C, \lambda, L) = -\log p(\mathbf{y} \mid \{h_c\}_{c=1}^C, \mathbf{x}_T)
\]  

(7)

The objective function from Eq. 3 becomes

\[
\frac{1}{G} \sum_{g=1}^G \sum_{j=1}^{J_g} \left( - (H\mathbf{x})^T y^{g,j} + B(f^{-1}(H\mathbf{x})) \right), \text{ s.t. } \mathbf{x}^g \geq 0, ||h_c||_2 = 1, \begin{cases}
||\mathbf{x}^g||_0 \leq \beta_0 \\
||\mathbf{x}^g||_1 \leq \beta_1
\end{cases}
\]  

(8)

Bernoulli generative model

We assume that we have access to data from $G$ neurons (groups). Each group consists of $J_g$ trials (observations) $y^{g,j} \in \{0,1\}$ that are binary time series. We model the entries from each of these as drawn from a Bernoulli likelihood with logit link function for $f(\cdot)$. Eq. 8 then becomes

\[
\frac{1}{G} \sum_{g=1}^G \sum_{j=1}^{J_g} \left( - (H\mathbf{x})^T y^{g,j} + 1 \right) \log \left( 1 + \exp \left( (H\mathbf{x})^T y^{g,j} \right) \right) - \lambda \sum_{g=1}^G \|h_c\|_2^2
\]  

(9)

with the working observation $\tilde{y}^{g,j} = y^{g,j} - (1 + \exp(-H\mathbf{x}^g))^{-1}$. Given this objective, ECOMP performs alternating minimization to learn $H$ and $\mathbf{x}^g$. For each group $g$, the encoder from DEA implements the following recurrence

\[
\mathbf{x}_T^g = \text{ReLU} \left( \frac{1}{L} \sum_{j=1}^{J_g} \tilde{y}^{g,j} - \lambda \right).
\]  

(10)

The auto-encoder architecture minimizes the loss function

\[
\mathcal{L}_H(\{y^{g,j}\}_{j=1}^{J_g}, \{h_c\}_{c=1}^C, \lambda, L) = - \left( \frac{1}{J_g} \sum_{j=1}^{J_g} y^{g,j} \right)^T (H\mathbf{x})^g + \frac{1}{J_g} \log \left( 1 + \exp \left( (H\mathbf{x})^g \right) \right).
\]  

(11)

Incorporating history dependence in the Bernoulli generative model

GLMs of neural spiking data [15] include a constant term that models the baseline probability of spiking, as well as a term that models the effect of spiking history. This motivates us to use the model

\[
\log \frac{p(y^{g,j} \mid \{h_c\}_{c=1}^C, \mathbf{x}^g, \mathbf{x}_T^g)}{1 - p(y^{g,j} \mid \{h_c\}_{c=1}^C, \mathbf{x}^g, \mathbf{x}_T^g)} = \mu^g + (H\mathbf{x})^g + \mathbf{Y}_j^g \mathbf{x}_T^g,
\]  

(12)

where the $n$th row of $\mathbf{Y}_j \in \mathbb{R}^{N \times K}$ contains the spiking history of neuron $g$ at trial $j$ going $K$ time steps prior to $n$, and $\mathbf{x}_T^g$ are coefficients that capture the effect of spiking history on the propensity of neuron $g$ to spike. We estimate $\mu^g$ from the average firing probability during the baseline period. The addition of the history term simply results in an additional set of variables to alternate over in the...
alternating-minimization interpretation of ECDL. We estimate it by adding a loop around ECOMP or backpropagation through DEA. Every iteration of this loop first assumes \( x^g_H \) are fixed. Then, it updates the filters and \( x^g \). Finally, it solves a convex optimization problem to update \( x^g_H \) given the filters and \( x^g \). In the interest of space, we do not describe this algorithm formally.

5 Results

Simulated neural spiking data We simulated neural spiking activity from \( G = 1,000 \) neurons according to Eq. 9. For each neuron \( g \), we simulated \( J_g = 60 \) trials each lasting 500 ms, i.e. \( y^{g,j} \in \mathbb{R}^{500} \). For a given neuron, each trial mimics the response of a barrel cortex neuron to two whisker deflections. The times when the whisker is deflected is the same for all 60 trials and occur randomly within the 500 ms interval but do not overlap. The whisker starts at a baseline position, is deflected with constant velocity in one direction for 25 ms, and then in the opposite direction with the same velocity and duration. We divided the data for each neuron into 30 trials for training and 30 trials for validation. Fig. 4(a) plots the whisker velocity in solid black. We used ECOMP and DEA to estimate the velocity of the whisker from the binary data. As is common in the CDL literature [22], we initialized both algorithms by randomly perturbing the true dictionary (gray, \( \Delta \)). The rationale behind this is two-fold. First, there exist methods [22] that provide good initializations. Second, in our application to real data, the application itself suggests a good choice of initialization. The figure demonstrates that both ECOMP (orange, \( \star \)) and DEA (green, \( \circ \)) are able to estimate the underlying whisker velocity accurately. Letting \( h_g \) denote an estimate of whisker velocity, we can measure the error between the true stimulus and an estimate using the standard measure [22] \( err(h_g, \hat{h}_g) = \sqrt{1 - (h_g, \hat{h}_g)^2} \), for \( \|h_g\| = \|\hat{h}_g\| = 1 \).

Fig. 4(b) shows that, as a function of iteration number (epoch), ECOMP converges faster compared to DEA. Intuitively, this is because the latter uses gradient style updates, while the former uses Newton’s method in the dictionary update step. Fig. 4(c) demonstrates the ability of both methods to identify the times when the whisker was deflected. Finally, Fig. 4(d) demonstrates that the encoders from DEA and ECOMP both perform sparse coding, namely identify the times when the whisker was deflected, significantly faster than CVXPY [23]. For instance, for 1,000 neurons, DEA and ECOMP are 70x and 4x faster than CVXPY respectively.

Figure 4: Results of applying the ECOMP and DEA to the simulated data. We refer the reader to the main text above for the interpretation of the results.

Real neural spiking data The dataset consists of neural spiking activity from \( G = 10 \) barrel cortex neurons in response to periodic whisker deflections. Each group \( g \) consists of \( J_g = 50 \) trials lasting 3000 ms, i.e. \( y^{g,j} \in \mathbb{R}^{3000} \). Each trial begins with a baseline period of 500 ms. During the following 2000 ms, a periodic deflection with period 125 ms is applied to a whisker identified as a primary whisker. The total number of deflections is 16, five of which are shown in Fig. 5. The stimulus represents whisker position. The trial ends with a baseline period of 500 ms. The blue curve in Fig. 6(a) depicts the velocity of whisker obtained as the first difference of the ideal whisker position programmed into the piezoelectrode used to deflect the whisker. The units are \( \frac{\text{mm}}{\text{ms}} \) per ms.

Previous work [20, 21] has demonstrated that one of key features of whisker motion encoded by barrel cortex neurons is whisker velocity. We applied DEA and ECOMP to these data. We let \( C = 1 \) and \( h_g \in \mathbb{R}^{125} \). We initialized the filter \( h_g \) using the whisker velocity stimulus (Fig. 6(a), blue). We set the sparsity level of ECOMP to \( \beta_0 = 16 \) and used \( \lambda = 0.119 \) for DEA. We used 30 trials from each neuron to learn \( h_1 \) and the remaining 20 trials as a test set to assess goodness of fit. We describe additional parameters used for DEA, as well as post-processing steps applied to it, in the Supplementary Material section.

The orange and green curves from Fig. 6(a) depict the estimates of whisker velocity computed from the neural spiking data using ECOMP and DEA respectively. The figure demonstrates that, within one period of whisker motion, whisker velocity, and therefore position, is similar to but deviates from the ideal motion programmed into the piezoelectric device used to move the whisker. In this experiment, the desired motion was to move the whisker in one direction and then in the opposite direction. The presence of peaks around 25, 60 and 100 ms suggest that, within one period, the whisker moved upwards multiple times, likely due to whisker motion with respect to the piezoelectrode. Fig. 6(b) depicts the 16 sparse codes that capture the effect of whisker velocity on neural spiking in each of the 16 deflection periods.
The heterogeneity of amplitudes estimated by DEA and ECOMP is indicative of the variability of the stimulus component of neural response across deflections. This is in sharp contrast to the GLM—detailed in the Supplementary Material section—which uses the ideal whisker velocity (Fig. 6(a), blue) as a covariate, and assumes that neural response to whisker deflections is constant across deflections.

In Fig. 6(c), we use the Kolmogorov-Smirnov (KS) test to compare how well the DEA, ECOMP and the GLM fit the data for a representative neuron in the dataset [24]. All three methods yield an estimate of the underlying intensity function of the neuron. KS plots are a visualization of the KS test for assessing the goodness of fit of models fit to point-process data, such as neural spiking data. We give a brief explanation of KS plots in the Supplementary Material section. The figure shows that DEA and ECOMP are a much better fit to the data than the GLM. The dotted lines represent 95% confidence intervals. Applied to the analysis of neural spiking data, the figure demonstrates that the proposed ECDL framework, which estimates the effect of stimuli from the data in an unsupervised fashion, is superior to GLM analyses based on user-defined covariates.

6 Conclusion
We introduced a general framework for learning a convolutional dictionary from data that are not real valued and drawn according to a distribution from the canonical exponential family. Through the connection between dictionary learning and auto-encoders, we showed how this framework translates into a principled prescription for training NNs using data that are not real valued. We applied both frameworks to the unsupervised learning of recurring convolutional patterns from neural spiking activity. Our results suggest that the proposed frameworks are superior to GLM analyses of neural data that rely on hand-crafted covariates.
A. ECOMP Algorithm

We describe the ECOMP algorithm for solving Eq. 3 in Algorithm 1. The superscript \( m \) refers to one iteration of the the alternating-minimization procedure, for \( m = 1, \ldots, M \). The subscript \( t \) refers to a single iteration of the encoder. The set \( S_t \) contains indices of the columns from \( \mathbf{H} \) that were chosen up to iteration \( t \). We call this set the active set in the main text. The notation \( \mathbf{H}_t \) refers to the \( t \)th column of \( \mathbf{H} \). The optimization problems in line 10 and 17 are both constrained convex optimization problems that can be solved using standard convex programming packages.

\[
\text{Algorithm 1: Exponential-family convolutional dictionary learning by ECOMP}
\]

\[
\text{Input: } \{y_j \}_{j=1}^{N}, \{h_n^{(0)} \}_{c=1}^{C} \in \mathbb{R}^K
\]

\[
\text{Output: } \{x^{(M)}_c \}_{c=1}^{C}, \{h^{(M)}_c \}_{c=1}^{C} \in \mathbb{R}^K
\]

1. for \( m = 1 \) to \( M \) do
2. (Convolutional Sparse Coding step)
3. for \( j = 1 \) to \( J \) do
4. \( S_0 = \emptyset, x_j^{(m-1)} = 0 \)
5. for \( t = 1 \) to \( T \) do
6. \( \tilde{y}_j = y_j - f^{-1}(H^{(m-1)}x_j^{(m-1)}) \)
7. \( c^*_t, n_t^* = \arg \max_{c,n} (h^{(m-1)}_c \ast \tilde{y}_j)[n] \in \mathbb{C}^{N-K+1} \)
8. \( i = c^*(N-K+1) + n^* \)
9. \( S_t = S_{t-1} \cup \{H_i^{(m-1)}\} \)
10. \( x_j^{(m)} = \arg \min_{x_j} \log p(y_j | \{h^{(m-1)}_c \}_{c=1}^{C}, x) \), s.t. \( x_j[n] \geq 0 \) for \( n \in S_t \)
11. \( x_j[n] = 0 \) for \( n \notin S_t \)
12. (Convolutional Dictionary Update step)
13. for \( j = 1 \) to \( J \) do
14. for \( c = 1 \) to \( C \) do
15. for \( i = 1 \) to \( N_i \) do
16. \( x_j^{(m)} = (0_{N_i \times K} \times x^{(m)}_i | n_j^{(0)}), \mathbf{I}_K \times K, 0_{(N-K-N_i^{(0)} \times K)} \)^T \)
17. \( \{h^{(m)}_c \}_{c=1}^{C} = \arg \min_{\{h_c \}_{c=1}^{C}} \sum_{j=1}^{J} \log p(y_j | \{h_c \}_{c=1}^{C}, \{x_j^{(m)}_c \}_{c,i,j=1}^{C}) \), s.t. \( \|h_c\|_2 = 1 \)

We found that ECOMP converged in \( M = 5 \) alternating-minimization iterations in the simulations, and \( M = 10 \) iterations in the analyses of the real data.

B. DEA Architecture

Algorithm 2 shows the forward pass of the DEA architecture. For notational convenience, we have dropped the superscript \( j \) indexing the \( J \) inputs.

\[
\text{Algorithm 2: DEA(y, h, } \lambda, \mathcal{L}) \text{: Forward pass of DEA architecture.}
\]

\[
\text{Input: } y, h, \lambda, \mathcal{L}
\]

\[
\text{Output: } w
\]

1. \( x_0 = 0 \)
2. for \( t = 1 \) to \( T \) do
3. \( x_t = \text{ReLU} (x_{t-1} + \frac{1}{\delta} \mathbf{H}^T (y - f^{-1}(Hx_{t-1})) - \frac{1}{\delta^2}) \)
4. \( w = Hx_T \)

Implementation of the DEA encoder We accelerate the computations performed by the DEA encoder by replacing ISTA with its faster version FISTA [25]. FISTA uses a momentum term to accelerate the converge of ISTA. The resulting encoder is similar to the one from [4]. We implemented the DEA architecture in Keras with Tensorflow as a backend. We trained it using backpropagation with the ADAM optimizer [26], along with AMSGrad [27], on an Nvidia GPU (GeForce GTX 1060). After training, the learned weights are the ones that minimize the validation loss.

Hyperparameters used for training the DEA architecture We set the regularization parameter \( \lambda = \sigma \sqrt{2 \log (C(N-K+1))} \). This choice is motivated by theoretical results for picking the regularization parameter for basis pursuit denoising [28]. We tuned \( \sigma \) by grid search in the interval of \([0.01, 0.3]\). Following the grid search, we used \( \sigma = 0.1 \) in the simulations and \( \sigma = 0.03 \) for the real data.
The DEA encoder performs $T = 250$ and $T = 5,000$ iterations of FISTA, respectively for the simulated and for the real data. We found that such large numbers, particularly for the real data, were necessary for the encoder to produce sparse codes. We used $L = 5$ in the simulations and $L = 2$ for the real data. We used batches of size 256 neurons in the simulations, and a single neuron per batch in the analyses of the real data.

**Processing of the output of the DEA encoder after training** The encoder of the DEA architecture performs $\ell_1$-regularized logistic regression using the convolutional dictionary $H$, the entries of which are highly correlated because of the convolutional structure. Suppose a group of observations $\{y_{g,j}\}_{j=1}^J$ are generated according to the Bernoulli generative model of Eq. 9 using a sparse vector $x_g$. We have observed that the estimate $x_{g,T}$ of $x_g$ obtained by feeding the group of observations to the DEA encoder is a vector whose nonzero entries are clustered around those of $x_g$. This is depicted in black in Fig. 7, and is a well-known issue with $\ell_1$-regularized regression with correlated dictionaries [29]. Therefore, after training the DEA architecture, we processed the output of the encoder as follows

1. Clustering: We applied k-means clustering to $x_{g,T}$ to identify 2 clusters and 16 clusters, respectively for the simulated and real data examples.

2. Support identification: For each cluster, we identified the index of the largest entry from $x_{g,T}$ in the cluster. This yielded a set of indices that correspond to the estimated support of $x_g$.

3. Logistic regression: We performed logistic regression using the group of observations and $H$ restricted to the support identified in the previous step. This yielded a new set of codes $x_g$ that were used to re-estimate $H$, similar to a single iteration of ECOMP.

The outcome of these three steps is shown in orange in Fig. 7.

![Figure 7: Output of the the DEA encoder before and after post-processing.](image)

**C. Generalized Linear Model (GLM) for Whisker Experiment**

We describe the GLM [15] used for analyzing the neural spiking data from the whisker experiment [21], and which we compared to ECOMP and DEA in Fig. 6. Fig. 5(b) depicts a segment of the periodic stimulus used in the experiment to deflect the whisker. The units are in mm. The full stimulus lasts 3000 ms and is equal to zero (whisker at rest) during the two baseline periods from 0 to 500 ms and 2500 to 3000 ms. In the GLM analysis, we used whisker velocity as a stimulus covariate, which corresponds to the first difference of the position stimulus $s \in \mathbb{R}^{3000}$. The blue curve in Fig. 6(a) represents one period of the whisker-velocity covariate. We associated a single stimulus coefficient $\beta_{\text{stim}} \in \mathbb{R}$ to this covariate. In addition to the stimulus covariate, we used history covariates in the GLM. We denote by $\beta_{g,H} \in \mathbb{R}^G$ the coefficients associated with these covariates, where $g = 1, \ldots, G$ is the neuron index. The GLM is given by

$$y_{g,j}[n] \sim \text{Bernoulli}(p_{g,j}[n])$$

s.t.  

$$p_{g,j}[n] = \left(1 + \exp\left(-\mu - \beta_{\text{stim}} \cdot (s[n] - k) - s[n-1-k] - \sum_{m=1}^{M_g} \beta_{g,H}[m] \cdot y_{g,j}[n-m]\right)\right)^{-1} \tag{13}$$
The parameters \( \{ \mu^g \}_{g=1}^G, \beta_{\text{stim}} \) and \( \{ \beta^g_{H} \}_{g=1}^G \) are estimated by minimizing the negative likelihood of the neural spiking data \( \{ y^{g,j} \}_{g,j=1}^{10,30} \) from all neurons using IRLS. We picked the order \( M_g \) (in ms) of the history effect for neuron \( g \) by fitting the GLM to each of the 10 neurons separately (i.e. \( \beta_{\text{stim}} = \beta^g_{\text{stim}} \)) and finding the value of \( 5 \leq M_g \leq 100 \) that minimizes the Akaike Information Criterion \([15]\).

### Interpretation of the GLM as a convolutional model

Because whisker position is periodic with period 125 ms, so is whisker velocity. Letting \( h_1 \) denote whisker velocity in the interval of length 125 ms starting at 500 ms (blue curve in Fig. 6(a)), we can interpret the GLM in terms of the convolutional model of Eq. 12. In this interpretation, \( H \) is the convolution matrix associated with the fixed filter \( h_1 \) (blue curve in Fig. 6(a)), and \( x^g \) is a sparse vector with 16 equally spaced nonzero entries all equal to \( \beta_{\text{stim}} \). The first nonzero entry of \( x^g \) occurs at index 500. The number of indices between nonzero entries is 125. The blue dots in Fig. 6(b) reflect this interpretation.

### D. Kolmogorov-Smirnov Plots and the Time-rescaling Theorem

Loosely, the time-rescaling theorem states that rescaling the inter-spike intervals (ISIs) of the neuron using the (unknown) underlying conditional intensity function (CIF) will transform them into i.i.d. samples from an exponential random variable with rate 1. This implies that, if we apply the CDF of an exponential random variable with rate 1 to the rescaled ISIs, these should look like i.i.d. draws from a uniform random variable in the interval \([0, 1]\). KS plots are a visual depiction of this result. They are obtained by computing the rescaled ISIs using an estimate of the underlying CIF and applying the CDF of an exponential random variable with rate 1 to them. These are then sorted and plotted against ideal uniformly-spaced empirical quantiles from a uniform random variable in the interval \([0, 1]\). The CIF that fits the data the best is the one that yields a curve that is the closest to the 45-degree diagonal. Fig. 6(c) depicts the KS plots obtained using the CIFs estimated using DEA, ECOMP and the GLM.
References

[1] Cristina Garcia-Cardona and Brendt Wohlberg. Convolutional dictionary learning: A comparative review and new algorithms. IEEE Transactions on Computational Imaging, 4(3):366–381, September 2018. There are errors in Equations (18) and (19) in the published version of the paper. These have been corrected in the most recent arXiv version.

[2] Yann LeCun, Yoshua Bengio, and Geoffrey Hinton. Deep learning. Nature, 521:436–444, 2015.

[3] Bahareh Tolooshams, Sourav Dey, and Demba Ba. Scalable convolutional dictionary learning with constrained recurrent sparse auto-encoders. In Proc. 2018 IEEE 28th International Workshop on Machine Learning for Signal Processing (MLSP), pages 1–6, Sept. 2018.

[4] Bahareh Tolooshams, Sourav Dey, and Demba Ba. Deep residual auto-encoders for expectation maximization-based dictionary learning, 2019. arXiv:1904.08827.

[5] Jeremias Sulam, Aviad Aberdam, Amir Beck, and Michael Elad. On multi-layer basis pursuit, efficient algorithms and convolutional neural networks. IEEE transactions on pattern analysis and machine intelligence, 2019.

[6] Pascal Vincent and Yoshua Bengio. Kernel matching pursuit. Machine Learning, 48(1):165–187, Jul 2002.

[7] Ac Lozano, Grzegorz Swirszcz, and Naoki Abe. Group orthogonal matching pursuit for logistic regression. Journal of Machine Learning Research, 15:452–460, 2011.

[8] Joseph Salmon, Zachary Harmany, Charles-Alban Deledalle, and Rebecca Willett. Poisson noise reduction with non-local pca. Journal of Mathematical Imaging and Vision, 48(2):279–294, Feb 2014.

[9] Raja Giryes and Michael Elad. Sparsity-based poisson denoising with dictionary learning. IEEE Transactions on Image Processing, 23(12):5057–5069, 2014.

[10] Ruslan Salakhutdinov, Andriy Mnih, and Geoffrey Hinton. Restricted boltzmann machines for collaborative filtering. In Proceedings of the 24th International Conference on Machine Learning, ICML ’07, pages 791–798, New York, NY, USA, 2007. ACM.

[11] P. McCullagh and J.A. Nelder. Generalized Linear Models. Chapman & Hall/CRC, 1989.

[12] Y. C. Pati, R. Rezaiifar, and P. S. Krishnaprasad. Orthogonal matching pursuit: recursive function approximation with applications to wavelet decomposition. In Proceedings of 27th Asilomar Conference on Signals, Systems and Computers, pages 40–44 vol.1, 1993.

[13] I. Daubechies, M. Defrise, and C. De Mol. An iterative thresholding algorithm for linear inverse problems with a sparsity constraint. Communications on Pure and Applied Mathematics, 57(11):1413–1457, 2004.

[14] Steven Diamond and Stephen Boyd. Cvxpy: A python-embedded modeling language for convex optimization. The Journal of Machine Learning Research, 17(1):2909–2934, 2016.

[15] Wilson Truccolo, Uri T Eden, Matthew Fellows, John Donoghue, and Emery N. Brown. A Point Process Framework for Relating Neural Spiking Activity to Spiking History, Neural Ensemble, and Extrinsic Covariate Effects. Journal of Neurophysiology, 93(2):1074–1089, 2005.

[16] Ludwig Fahrmeir and Gerhard Tutz. Multivariate statistical modelling based on generalized linear models. Springer Science & Business Media, 2013.

[17] Donghui Chen and Robert J. Plemmons. Nonnegativity constraints in numerical analysis. In The Birth Of Numerical Analysis, pages 109–139. World Scientific Publishing Co. Pte. Ltd., 2010.

[18] R. Byrd, P. Lu, J. Nocedal, and C. Zhu. A limited memory algorithm for bound constrained optimization. SIAM Journal on Scientific Computing, 16(5):1190–1208, 1995.

[19] John R. Hershey, Jonathan Le Roux, and Felix Weninger. Deep unfolding: Model-based inspiration of novel deep architectures. arXiv:1309.2574 [cs.LG], pages 1–27, 2014.

[20] Simona Temereanca, Emery N. Brown, and Daniel J. Simons. Rapid changes in thalamic firing synchrony during repetitive whisker stimulation. Journal of Neuroscience, 28(44):11153–11164, 2008.

[21] Demba Ba, Simona Temereanca, and Emery Brown. Algorithms for the analysis of ensemble neural spiking activity using simultaneous-event multivariate point-process models. Frontiers in Computational Neuroscience, 8:6, 2014.

[22] Alekh Agarwal, Anima Anandkumar, Prateek Jain, Praneeth Netrapalli, and Rashish Tandon. Learning sparsely used overcomplete dictionaries via alternating minimization. SIAM Journal on Optimization, 26:2775–2799, 2016.
[23] Steven Diamond and Stephen Boyd. CVXPY: A Python-embedded modeling language for convex optimization. *Journal of Machine Learning Research*, 17(83):1–5, 2016.

[24] Emery N. Brown, Riccardo Barbieri, Valérie Ventura, Robert E. Kass, and Loren M. Frank. The time-rescaling theorem and its application to neural spike train data analysis. *Neural Computation*, 14(2):325–346, 2002.

[25] Amir Beck and Marc Teboulle. A fast iterative shrinkage-thresholding algorithm for linear inverse problems. *SIAM Journal on Imaging Sciences*, 2(1):183–202, 2009.

[26] Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *Proc. the 3rd International Conference on Learning Representations (ICLR)*, pages 1–15, 2014.

[27] Sashank J. Reddi, Satyen Kale, and Sanjiv Kumar. On the convergence of adam and beyond. In *Proc. International Conference on Learning Representations*, pages 1–23, 2018.

[28] Scott Saobing Chen, David L. Donoho, and Michael A. Saunders. Atomic decomposition by basis pursuit. *SIAM Review*, 43:129–159, 1998.

[29] Badri Narayan Bhaskar, Gongguo Tang, and Benjamin Recht. Atomic norm denoising with applications to line spectral estimation. *IEEE Transactions on Signal Processing*, 61(23):5987–5999, 2013.