

Neural Network Reconstruction via Graph Locality-Driven Machine Learning

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Abstract

A consistent problem within the field of computational neuroscience is the determination of biological neural network structure and connectivity from imaging of stochastic, large-scale network activity. We propose a machine learning algorithm inspired by convolutional approaches to image processing, adapted to the graph structure of neural networks. To achieve this, we redefine locality in terms of graph adjacency, and create a scale-indepent algorithm facilitated by modern machine learning techniques to incorporate this locality data into individual connection prediction.

1 Background

1.1 Biological Neural Networks

1.2 Graph Structures

1.2.1 Graph Locality

1.3 Convolutional Neural Networks

1.4 Concepts and Terms

Before diving into the specifics of data production, model architecture, and training, it's important to establish several important concepts.

1.4.1 Adjacency Matrices

The representation of neural network connectivity that we will focus on is the adjacency matrix. For n neurons, an adjacency matrix \mathbb{M} will be of dimensions $(n \times n)$. A simplistic method of predicting network activity, and one that we will use to produce our data, is to multiply this matrix by an n -vector representing current activity at each neuron. Such an operation appears as

follows for $n = 3$:

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} \times \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} ax + by + cz \\ dx + ey + fz \\ gx + hy + iz \end{bmatrix}$$

Thus the activity for a given neuron is defined entirely in terms of network activity at the previous timestep and the weights in the adjacency matrix in the row corresponding to that neuron. We thereby arrive at a simple expression of the mechanics of adjacency matrices:

1. Weights in some row i define inputs to neuron i
2. Weights in some column j define outputs from neuron j
3. The singular weight at \mathbb{M}_{ij} defines the connection from neuron j to neuron i .

Keeping this inverse relationship in mind will help prevent confusion in later chapters.

2 Model

The model trained and tested here represents ... stuff

2.1 Data

Insofar as we treat ANNs as providing arbitrary function approximation, training a network requires input data representing the known data about the system we wish to model, as well as output data we wish the network to produce from the inputs. More generally, input data usually entails information that is easy to acquire about the process being modeled, while output data, or labels, correspond to a dataset that is difficult to acquire generally. Of course, this means that the first step in training a neural network is to assemble a sufficiently large set of inputs and outputs in order to fully, or at least approximately, characterize the problem at hand.

In our case, we wish to map from (relatively) easily available data about biological networks, individual neuron spike times, to network structure. While such data exist, generating our own allows us to better analyze the results of the algorithm.

2.1.1 Generation

In order to demonstrate the validity of our algorithm for graph convolution, we opt for a simplified form of the kind of data that would be used in a real-world setting. To this end, we create adjacency matrices representing simple, small- n toy networks.

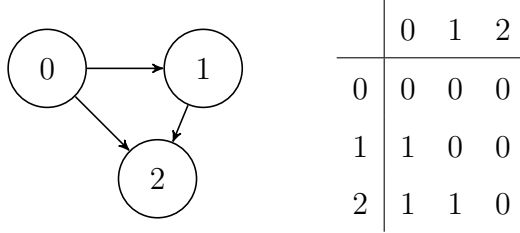


Figure 2.1: Example of 3-neuron network and adjacency matrix.

Binary values are used throughout these toy networks: either a connection exists or it doesn't; either a 'neuron' is spiking or it isn't. To produce spiking data, we create an n -vector \mathbb{S} representing the current state of the toy network, with random neurons already spiking based on a chosen spike rate. From here, the process is as in 1.4.1, where \mathbb{M} is the adjacency matrix:

$$\underset{n \times n}{\mathbb{M}} \times \underset{n \times 1}{\mathbb{S}^t} = \underset{n \times 1}{\mathbb{S}^{t+1}}$$

Additionally, \mathbb{S}^{t+1} may have one or more neurons spike randomly, as determined by the spike rate of the simulation.¹ All values are clipped to the range $[0, 1]$, to avoid double spiking.

At each step, \mathbb{S} is appended to an output matrix, which is saved after simulation is complete. For t simulation steps, the completed output has shape $(n \times t)$.

¹SEE APPENDIX

Example Data Generation

Consider the network defined in figure 2.1. Supposing that we randomly spike neuron 0 at the first step, our initial state appears as such, where \mathbb{O} is the output matrix and \mathbb{R}^0 is an n -vector wherein each element has been randomly assigned 0 or 1, based on the spike rate of the simulation:

$$\mathbb{M} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix} \quad \mathbb{S}^0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \mathbb{O} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \mathbb{R}^0 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

We now compute \mathbb{S}^1 as above:

$$\mathbb{S}^1 = (\mathbb{M} \times \mathbb{S}^0) + \mathbb{R}^0 = \left(\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}$$

In this case, neuron 1 was spiked randomly, but was also spiked by virtue of its connection from 0. Since in this simple model we only consider neurons to be either spiking or not, binary values, we clip the values in \mathbb{S}^1 to a maximum of 1, in order to prevent cases such as this one from causing spikes of greater magnitude to propagate through the network. This also prevents neurons from double spiking due to multiple inputs being active in the same timestep. Thus we have our final value for \mathbb{S}^1 , and append it to \mathbb{O} .

$$\mathbb{S}^1 = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \quad \mathbb{O} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

If we were to repeat this process several more times, we might end up with an output matrix such as in figure 2.2.

$$\mathbb{O} = [\mathbb{S}^0 \mid \mathbb{S}^1 \mid \mathbb{S}^2 \mid \mathbb{S}^3 \mid \mathbb{S}^4] = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

Figure 2.2: Example output matrix for a 3-neuron network simulated for five steps.

We can clearly see the effects of neuron 2 having inputs from both other neurons. Practically, the number of iterations was usually set to 50.

2.1.2 Restructuring

The model accepts data in the form of a spike-time raster plot of dimensions $(n \times t)$, where n is the number of neurons and t is the number of timesteps being considered. The axes are reversed in comparison to the data created by the generator, and thus in the process of loading in the spike trains we transpose the matrices to the expected dimensionality. Additionally, it is not always necessary to use the full number of steps generated, depending on the size of the generator network in question, as well as its spike rate. In such a scenario, we truncate the time dimension appropriately.

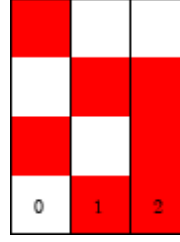
For a network accepting t timesteps of data from n neurons, the data fed into the network takes the following form:

$$\begin{bmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{t1} & x_{t2} & \dots & x_{tn} \end{bmatrix}$$

Applying this process to the data in figure 2.2, including truncating the time dimension to four, results in the following:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

(a) Transposed output matrix



(b) Graphical representation

Figure 2.3: Transposed and truncated matrix and associated visualization.

The representation of the matrix in 2.3b is an example of the method we will use to depict matrices containing real values.

2.1.3 Generalizability

In most ANN implementations, feeding various data with the same label attached to it results in the network learning to ignore the input data and always return the desired label, rendering it useless. However, due to the unique structure of our model, this sort of overfitting is impossible (SEE SOME ARCHITECTURE SECTION). Therefore, we must merely construct a suitably representative generator network, meaning that it contains all of the inter-neuron relationships we expect to see in the data we ultimately feed in to test.

2.2 Architecture

We will first describe the architecture in terms that, while accurate on the macro level, do not fully reflect the actual transformations occurring in the implemented model. We will then proceed to a mathematically representative

version, leaving explanation of the batched version of the model to APPENDIX SECTION.

2.2.1 Structure & Computation Details

Dimensionality-defining Variables

Only two values characterize the matrices and transitions involved in the model. They are as follows:

b : The number of steps of input data the model considers in a given segment of data.

d : The length of the vectors characterizing each potential connection ij . This restricts the maximum information about each potential neuron pair that the model can maintain across layer transitions.

We determined effective values for these parameters through experimentation.

Additionally, we use the number of nodes in the generator graph, n , to calculate summations and averages, but the structure of our calculations is such that no aspects of the model are defined in terms of n .

Activation Functions

At the end of each transition, an elementwise activation function² is applied following completion of all computations. For all but the final layer, that function is ReLU³, which is defined as follows:

$$relu(x) = \begin{cases} 0 & x < 0 \\ x & x \geq 0 \end{cases} \quad (2.1)$$

²SEE THE PART OF THE BG WHERE I TALK ABOUT NN PRINCIPLES

³NEEDS CITATION

2.2.2 First Transition

To generate the first layer of the network, we inspect every pair of neurons in the input data. Since no pair of neurons is distinguishable from another, the comparison applied is the same in all cases: we apply the same convolutional filter to all pairs. We achieve this by concatenating the spike train of each neuron i individually with every other neuron j , then multiplying by a matrix \mathbb{W} of dimensionality $(d \times 2b)$.⁴

\mathbb{W} is trained on, and thus the comparison of each pair of spike trains is left up to the network. The transition appears as follows, where \mathbb{I}_x is the input column at x :

$$\forall i, j \mid 0 \leq i, j < n : d'_{ij} = \underset{d \times 1}{\mathbb{W}} \times \underset{d \times 2b}{\left(\frac{\mathbb{I}_i}{\mathbb{I}_j} \right)}$$

This leaves us with n^2 d -vectors, each characterizing one potential edge ij .

2.2.3 Convolutional Layer

In this layer, we incorporate information from all nodes potentially adjacent to each edge ij . From our previous layer, we have a matrix of shape $(d \times n^2)$ that we will refer to as \mathbb{D}' , but it will be useful to keep in mind an alternate representation of that matrix, one in three dimensions, which we shall refer to as \mathbb{D}'_N . This transformation is demonstrated in figure 2.4.

⁴Recall that the time dimension fed into the network is characterized by b .

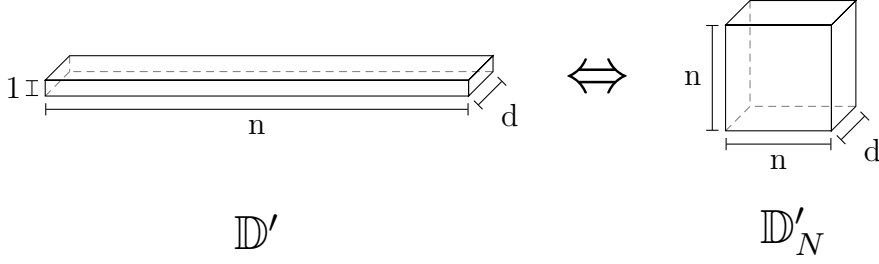


Figure 2.4: Relationship between \mathbb{D}' and \mathbb{D}'_N .

Consider some d'_{ij} in \mathbb{D}'_N . Then we can say the following:

1. d'_{ij} represents the connection from j to i as it may or may not exist in this network, in the form of d values of indeterminate meaning
2. $\forall k \mid 0 \leq k < n$, d'_{jk} represents a potential input to j
3. $\forall k \mid 0 \leq k < n$, d'_{ki} represents a potential output from i

In our determination of the presence or absence of a connection from j to i , we wish to incorporate information from these potentially connected nodes; i.e., these inputs and outputs represent potential neighbors in terms of graph locality. To achieve this, we perform the following computations⁵ for each d_{ij} :

$$\mathbb{I}_{d \times 1} = \frac{1}{n} \sum_{k=0}^{n-1} d'_{jk} \quad \mathbb{O}_{d \times 1} = \frac{1}{n} \sum_{k=0}^{n-1} d'_{ki} \quad (2.2a)$$

$$\mathbb{I}_{\mathbb{D}} = \mathbb{W}'_{in} \times (\mathbb{I} \odot d'_{ij}) \quad \mathbb{O}_{\mathbb{D}} = \mathbb{W}'_{out} \times (\mathbb{O} \odot d'_{ij}) \quad (2.2b)$$

Here we arrive at the output, d''_{ij} :

$$d''_{ij} = \mathbb{W}'_{tot} \times \begin{pmatrix} \mathbb{I}_{\mathbb{D}} \\ \mathbb{O}_{\mathbb{D}} \end{pmatrix} \quad (2.2c)$$

⁵Actually, it's much more elegant.

Conceptually, in **(2.2a)** we first average all potential inputs to and outputs from potential edge ij . Then, we compute an entrywise product (\odot) of these vectors with the vector describing the edge in question, d''_{ij} . While we have integrated locality data into the results thus far, the network has not been allowed any processing over the resultant data, which we rectify by multiplying the input and output vectors with separate dimensionality-preserving ($d \times d$) matrices. We thus arrive at **(2.2b)**, with vectors $\mathbb{I}_{\mathbb{D}}$ and $\mathbb{O}_{\mathbb{D}}$ representing edge ij with inputs and outputs, respectively, taken into consideration. In **(2.2c)**, we arrive at d''_{ij} as it will be seen by the next layer of the network by multiplying a third weight matrix by the vertical concatenation of $\mathbb{I}_{\mathbb{D}}$ and $\mathbb{O}_{\mathbb{D}}$. This matrix \mathbb{W}'_{tot} , allows the network to optimize for whichever elements in $\mathbb{I}_{\mathbb{D}}$ and $\mathbb{O}_{\mathbb{D}}$ are most important in the prediction of ij . The three matrices involved, \mathbb{W}'_{in} , \mathbb{W}'_{out} , and \mathbb{W}'_{tot} , are trained on by the optimizer⁶, allowing the model to learn optimal processing and combinations to facilitate predictions.

Our concatenation approach in **(2.2c)** stands in contrast to the strategy taken in **(2.2b)**, where integration of the input and output data is forced via entrywise product computation. While we considered the same concatenation process for use in **(2.2b)**, the apparent difficulty of integrating the calculated locality data into the prediction of ij led the model to rapidly adapt its weight matrices to ignore the locality portion of the data. For more discussion on this difficulty, see TRAINING SECTION.

Note again that none of the computations involved in this layer are dependent on n ; as the summations are averaged, the values contained in their resultant vectors will be of similar magnitude for any number of neurons under consideration. After executing this algorithm for each d''_{ij} , we are left with

⁶SEE OPTIMIZER SECION IN TRAINING

another $(d \times n^2)$ output matrix, \mathbb{D}'' .

2.2.4 Final Transition

The shift from $(d \times n^2)$ is comparatively simple, being only a dimensionality reduction:

$$\forall d''_{ij} \in \mathbb{D}'' : d''_{ij} = \underset{1 \times 1}{\mathbb{W}^f} \times \underset{d \times 1}{d''_{ij}} \quad (2.3)$$

This leaves us with a $(1 \times n^2)$ matrix, which, following application of a hyperbolic tangent activation function and transposition to $(n \times n)$, we treat as the adjacency matrix of the generator associated with the input data.

3 Training

3.1 Datasets

3.2 Matrix Initialization

3.3 Hyperparameter Optimization

3.3.1 Loss Optimization

Loss Function

Optimizer Function

4 Results

4.1 3-neuron generator

We first consider a generator network consisting of three nodes connected as in figure 4.1. All weights are binary, and a spike rate of .25 was used.¹

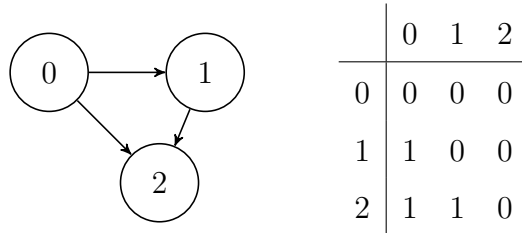


Figure 4.1: Network structure and adjacency matrix of the generator. (Reproduced from Figure 2.1)

While reconstructing a graph comprising only three nodes is not much of a feat, this simplified case allows us to demonstrate that our convolutional approach is capable of reconstruction at all. Furthermore, the small network size requires few timesteps and a small interlayer featurespace; i.e., $b, d < 10$. This results in a relatively simple set of transitions, allowing us to explore and understand the inner workings of the network.

¹SEE APPENDIX for information on spike rates

4.1.1 Example Model

The following data are pulled from a model trained on data produced by the generator in figure 4.1. Figure 4.2 demonstrates the model’s loss over time. In this example, b and d were pushed down in order to allow for better comprehension of the internal mechanics; the loss tends to converge more effectively and evenly given more computation power.

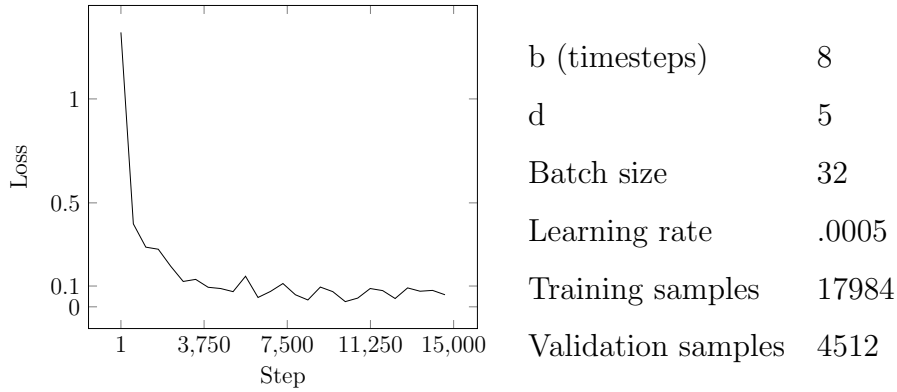


Figure 4.2: Training loss and parameters for model described in 4.1.1

Trained Network Operation

Here, we examine in brief the internal operation of the trained model over a single input. For a complete look through the procedure of reconstruction for this network, please see APPENDIX.

The last transformation of the network involves a matrix multiplication of the final layer weights² with the data in 4.3c. This produces the adjacency matrix found in figure 4.4.

²see appendix

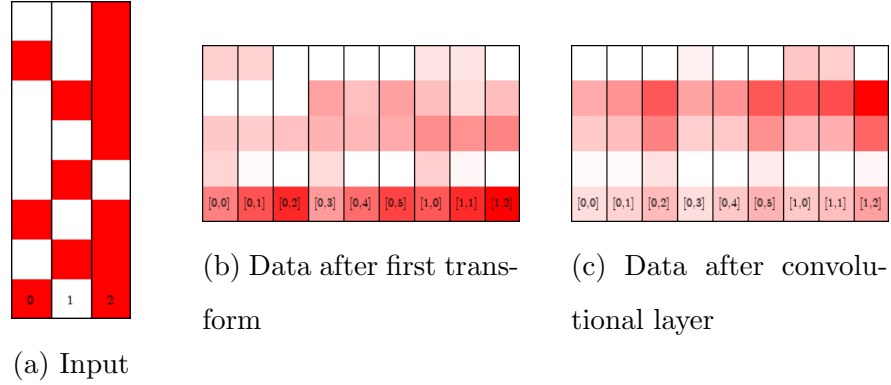


Figure 4.3: Path of data through network, up to final transform

	0	1	2
0	.02	.03	.01
1	.99	.01	-.01
2	1.00	1.00	.02

Figure 4.4: Output for input data in figure 4.3a

4.2 Applicability Beyond Training Data

As described in ??, the fact that our model is trained on data produced by only one generator is of little consequence; due to its structure, the only information it can learn is relational; i.e., per-neuron-pair. Consider the following examples, in which data was produced from several generator networks and fed into the model described in 4.1:

TODO: add examples of input and output data to 3.2.1 and 3.2.2.

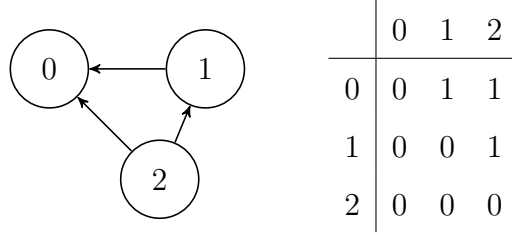
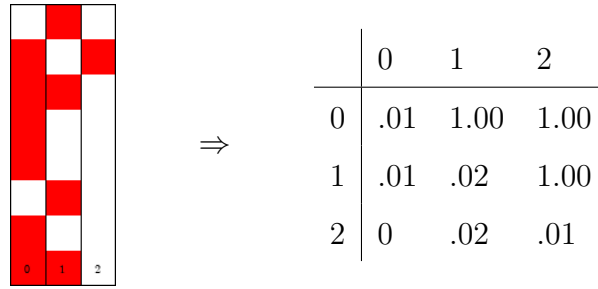


Figure 4.5: Inverted version of figure 4.1

4.2.1 Inverted Network

Despite being a complete inversion of the generator used to train the model in 4.1, reconstruction of this network is simple.



4.2.2 Cyclical Network

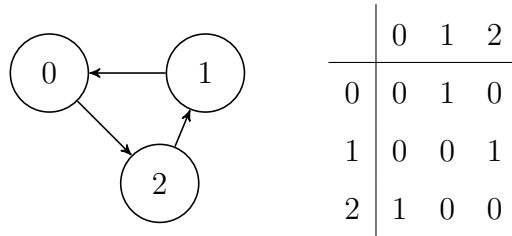


Figure 4.6: Cyclical 3-neuron network

For a cyclical network, the situation is not quite so simple. Due to the perpetual propagation of spikes through the generator, additional random spiking

can cause the input data to become an impenetrable mess. Tempering the spike rate to 0.05 produces workable data, but the results are neither so clean nor consistent as for terminating networks.

A Parameter Optimization Miscellaneous

A.1 Data

A.1.1 Spike Rate Determination

As seen in section 4.2.2, oversaturated data hampers the ability of our model to perform accurate reconstructions. As the

B Model

B.1 Batched Architecture Calculations