

# Interrogating theoretical models of neural computation with deep inference

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## <sup>1</sup> 1 Abstract

<sup>2</sup> The cornerstone of theoretical neuroscience is the circuit model: a system of equations that captures  
<sup>3</sup> a hypothesized neural mechanism. Such models are valuable when they give rise to an experimen-  
<sup>4</sup> tally observed phenomenon – whether behavioral or in terms of neural activity – and thus can offer  
<sup>5</sup> insights into neural computation. The operation of these circuits, like all models, critically depends  
<sup>6</sup> on the choices of model parameters. Historically, the gold standard has been to analytically derive  
<sup>7</sup> the relationship between model parameters and computational properties. However, this enterprise  
<sup>8</sup> quickly becomes infeasible as biologically realistic constraints are included into the model increas-  
<sup>9</sup> ing its complexity, often resulting in *ad hoc* approaches to understanding the relationship between  
<sup>10</sup> model and computation. We bring recent machine learning techniques – the use of deep generative  
<sup>11</sup> models for probabilistic inference – to bear on this problem, learning distributions of parameters  
<sup>12</sup> that produce the specified properties of computation. Importantly, the techniques we introduce  
<sup>13</sup> offer a principled means to understand the implications of model parameter choices on compu-  
<sup>14</sup> tational properties of interest. We motivate this methodology with a worked example analyzing  
<sup>15</sup> sensitivity in the stomatogastric ganglion. We then use it to generate insights into neuron-type  
<sup>16</sup> input-responsivity in a model of primary visual cortex, a new understanding of rapid task switch-  
<sup>17</sup> ing in superior colliculus models, and attribution of bias in recurrent neural networks solving a toy  
<sup>18</sup> mathematical problem. More generally, this work offers a quantitative grounding for theoretical  
<sup>19</sup> models going forward, pointing a way to how rigorous statistical inference can enhance theoretical  
<sup>20</sup> neuroscience at large.

## <sup>21</sup> 2 Introduction

<sup>22</sup> The fundamental practice of theoretical neuroscience is to use a mathematical model to understand  
<sup>23</sup> neural computation, whether that computation enables perception, action, or some intermediate  
<sup>24</sup> processing [1]. In this field, a neural computation is systematized with a set of equations – the  
<sup>25</sup> model – and these equations are motivated by biophysics, neurophysiology, and other conceptual  
<sup>26</sup> considerations. The function of this system is governed by the choice of model parameters, which

27 when configured appropriately, give rise to a measurable signature of a computation. The work of  
28 analyzing a model then requires solving the inverse problem: given a computation of interest, how  
29 can we reason about these suitable parameter configurations? The inverse problem is crucial for  
30 reasoning about likely parameter values, uniquenesses and degeneracies, attractor states and phase  
31 transitions, and predictions made by the model.

32 Consider the idealized practice: one carefully designs a model and analytically derives how model  
33 parameters govern the computation. Seminal examples of this gold standard include our field's  
34 understanding of memory capacity in associative neural networks [2] and chaos and autocorrelation  
35 timescales in random neural networks [3] (which use models and analyses originating in physics),  
36 as well as the paradoxical effect in excitatory/inhibitory networks [4], we need [?], more examples  
37 [?]. Unfortunately, as circuit models include more biological realism, theory via analytic derivation  
38 becomes intractable. This creates an unfavorable tradeoff. On the one hand, one may tractably  
39 analyze systems of equations with unrealistic assumptions (for example symmetry or gaussianity),  
40 producing accurate inferences about parameters of a too-simple model. On the other hand, one may  
41 choose a more biologically accurate, scientifically relevant model at the cost of *ad hoc* approaches  
42 to analysis (simply examining simulated activity), potentially resulting in bad inferences and thus  
43 erroneous scientific predictions and conclusions.

44 Of course, this same tradeoff has been confronted in many scientific fields and engineering problems  
45 characterized by the need to do inference in complex models. In response, the machine learning  
46 community has made remarkable progress in recent years, via the use of deep neural networks as  
47 a powerful inference engine: a flexible function family that can map observed phenomena (in this  
48 case the measurable signal of some computation) back to probability distributions quantifying the  
49 likely parameter configurations. One celebrated example of this approach from machine learning, of  
50 which we draw key inspiration for this work, is the variational autoencoder [5, 6], which uses a deep  
51 neural network to induce an (approximate) posterior distribution on hidden variables in a latent  
52 variable model, given data. Indeed, these tools have been used to great success in neuroscience as  
53 well, in particular for interrogating parameters (sometimes treated as hidden states) in models of  
54 both cortical population activity [7, 8, 9, 10] and animal behavior [11, 12, 13]. These works have  
55 used deep neural networks to expand the expressivity and accuracy of statistical models of neural  
56 data [14].

57 However, these inference tools have not significantly influenced the study of theoretical neuroscience  
58 models, for at least three reasons. First, at a practical level, the nonlinearities and dynamics of

many theoretical models are such that conventional inference tools typically produce a narrow set of insights into these models. Indeed, only in the last few years has deep learning research advanced to a point of relevance to this class of problem. Second, the object of interest from a theoretical model is not typically data itself, but rather a qualitative phenomenon – inspection of model behavior, or better, a measurable signature of some computation – an *emergent property* of the model. Third, because carefully constructed biological models do not fit cleanly into the framing of a statistical model. Technically, because many such models stipulate a noisy system of differential equations that can only be sampled or realized through forward simulation, they lack the explicit likelihood and priors central to the probabilistic modeling toolkit.

To address these three challenges, we developed an inference methodology – ‘emergent property inference’ – which learns a distribution over parameter configurations in a theoretical model. This distribution has two critical properties: *(i)* it is chosen such that draws from the distribution (parameter configurations) correspond to systems of equations that give rise to a specified emergent property (a set of constraints); and *(ii)* it is chosen to have maximum entropy given those constraints, such that we identify all likely parameters and can use the distribution to reason about parametric sensitivity and degeneracies [15]. First, we stipulate a bijective deep neural network that induces a flexible family of probability distributions over model parameterizations with a probability density we can calculate [16, 17, 18]. Second, we quantify the notion of emergent properties as a set of moment constraints on datasets generated by the model. Thus, an emergent property is not a single data realization, but a phenomenon or a feature of the model, which is ultimately the object of interest in theoretical neuroscience. Conditioning on an emergent property requires a variant of deep probabilistic inference methods, which we have previously introduced [19]. Third, because we cannot assume the theoretical model has explicit likelihood on data or the emergent property of interest, we use stochastic gradient techniques in the spirit of likelihood free variational inference [20]. Taken together, emergent property inference (EPI) provides a methodology for inferring parameter configurations consistent with a particular emergent phenomena in theoretical models. We use a classic example of parametric degeneracy in a biological system, the stomatogastric ganglion [21], to motivate and clarify the technical details of EPI.

Equipped with this methodology, we then investigated three models of current importance in theoretical neuroscience. These models were chosen to demonstrate generality through ranges of biological realism (from conductance-based biophysics to recurrent neural networks), neural system function (from pattern generation to abstract cognitive function), and network scale (from four to

91 infinite neurons). First, we use EPI to produce a set of verifiable hypotheses of input-responsivity  
 92 in a four neuron-type dynamical model of primary visual cortex; we then validate these hypotheses  
 93 in the model. Second, we demonstrated how the systematic application of EPI to levels of task  
 94 performance can generate experimentally testable hypotheses regarding connectivity in superior  
 95 colliculus. Third, we use EPI to uncover the sources of bias in a low-rank recurrent neural network  
 96 executing a toy mathematical computation. The novel scientific insights offered by EPI contextualize  
 97 and clarify the previous studies exploring these models [22, 23, 24, 25] and more generally,  
 98 suggests a departure from realism vs tractability considerations towards the use of modern machine  
 99 learning for sophisticated interrogation of biologically relevant models.

100 We note that, during our preparation and early presentation of this work [26, 27], another work  
 101 has arisen with broadly similar goals: bringing statistical inference to mechanistic models of neural  
 102 circuits [28]. We are excited by this broad problem being recognized by the community, and we  
 103 emphasize that these works offer complementary neuroscientific contributions and use different  
 104 technical methodologies. While we have advanced our research on deep generative modeling [19]  
 105 to a point of significant relevance to statistical inference in theoretical neuroscience, they have  
 106 also furthered their research on approximate Bayesian inference in such models [29].  
 107 The existence of these complementary methodologies emphasizes the increased importance and  
 108 timeliness of both works.

## 109 3 Results

### 110 3.1 Motivating emergent property inference of theoretical models

111 Consideration of the typical workflow of theoretical modeling clarifies the need for emergent prop-  
 112 erty inference. First, one designs or chooses an existing model that, it is hypothesized, captures  
 113 the computation of interest. To ground this process in a well-known example, consider the stom-  
 114 atogastric ganglion (STG) of crustaceans, a small neural circuit which generates multiple rhythmic  
 115 muscle activation patterns for digestion [30]. Despite full knowledge of STG connectivity and a  
 116 precise characterization of its rhythmic pattern generation, biophysical models of the STG have  
 117 complicated relationships between circuit parameters and neural activity [21, 31]. A model of the  
 118 STG [22] is shown schematically in Figure 1A, and note that the behavior of this model will be crit-  
 119 ically dependent on its parameterization – the choices of conductance parameters  $z = [g_{el}, g_{synA}]$ .  
 120 Specifically, the two fast neurons ( $f_1$  and  $f_2$ ) mutually inhibit one another, and oscillate at a

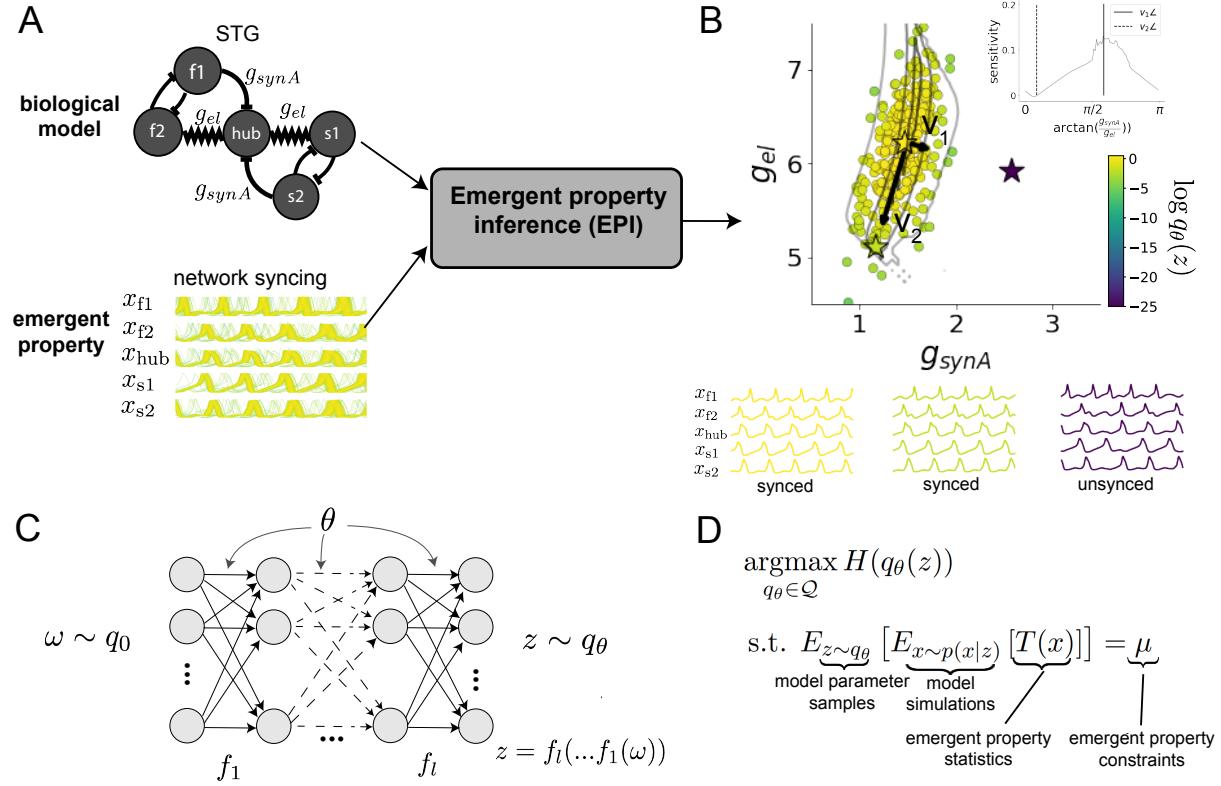


Figure 1: Emergent property inference (EPI) in the stomatogastric ganglion. A. For a choice of model (STG) and emergent property (network syncing), emergent property inference (EPI) learns a posterior distribution of the model parameters  $z = [g_{el}, g_{synA}]^\top$  conditioned on network syncing. B. An EPI distribution of STG model parameters producing network syncing. Samples are colored by log density. Distribution contours of emergent property value error are shown at levels of  $2 \times 10^{-6}$ ,  $2 \times 10^{-5}$ , and  $2 \times 10^{-4}$ . The eigenvectors of the Hessian at the mode of the inferred distribution are indicated as  $v_1$  and  $v_2$ . Simulated activity is shown for three samples (stars). (Inset) Sensitivity of the system with respect to network syncing along all dimensions of parameter space away from the mode. (see Section A.2.1). C. Deep probability distributions map a latent random variable  $w$  through a deep neural network with weights and biases  $\theta$  to parameters  $z$  distributed as  $q_\theta(z)$ . D. EPI learns a distribution  $q_\theta(z)$  of model parameters that produce an emergent property: the emergent property statistics  $T(x)$  are fixed in expectation over parameter distribution samples  $z \sim q_\theta(z)$  to particular values  $\mu$ .

121 faster frequency than the mutually inhibiting slow neurons ( $s_1$  and  $s_2$ ), and the hub neuron (hub)  
122 couples with the fast or slow population or both.

123 Second, once the model is selected, one defines the emergent property, the measurable signal of  
124 scientific interest. To continue our running STG example, one such emergent property is the  
125 phenomenon of *network syncing* – in certain parameter regimes, the frequency of the hub neuron  
126 matches that of the fast and slow populations at an intermediate frequency. This emergent property  
127 is shown in Figure 1A at a frequency of 0.54Hz.

128 Third, qualitative parameter analysis ensues: since precise mathematical analysis is intractable in  
129 this model, a brute force sweep of parameters is done [22]. Subsequently, a qualitative description is  
130 formulated to describe of the different parameter configurations that lead to the emergent property.  
131 In this last step lies the opportunity for a precise quantification of the emergent property as a  
132 statistical feature of the model. Once we have such a methodology, we can infer a probability  
133 distribution over parameter configurations that produce this emergent property.

134 Before presenting technical details (in the following section), let us understand emergent property  
135 inference schematically: EPI (Fig. 1A gray box) takes, as input, the model and the specified  
136 emergent property, and as its output, produces the parameter distribution shown in Figure 1B.  
137 This distribution – represented for clarity as samples from the distribution – is then a scientifically  
138 meaningful and mathematically tractable object. In the STG model, this distribution can be  
139 specifically queried to reveal the prototypical parameter configuration for network syncing (the  
140 mode; Figure 1B yellow star), and how network syncing decays based on changes away from the  
141 mode. Intuitively, the probability density of the samples is in agreement with the emergent property  
142 value error (Fig. 1B contours). Furthermore, the eigenvectors of the distribution Hessian at the  
143 mode can be queried to quantitatively formalize the robustness of network syncing (Fig. 1B  $v_1$ ,  
144  $v_2$ ). Indeed, samples equidistant from the mode along these EPI-identified dimensions of sensitivity  
145 ( $v_1$ ) and degeneracy ( $v_2$ ) have diminished or preserved network syncing, respectively (Figure 1B  
146 inset and activity traces). Further validation of EPI is available in the supplementary materials,  
147 where we analyze a simpler model for which ground-truth statements can be made (Section A.1.1).

## 148 3.2 A deep generative modeling approach to emergent property inference

149 Emergent property inference (EPI) systematizes the three-step procedure of the previous section.  
150 First, we consider the model as a coupled set of differential (and potentially stochastic) equations

[22]. In the running STG example, the dynamical state  $x = [x_{f1}, x_{f2}, x_{hub}, x_{s1}, x_{s2}]$  is the membrane potential for each neuron, which evolves according to the biophysical conductance-based equation:

$$C_m \frac{dx}{dt} = -h(x; z) = -[h_{leak}(x; z) + h_{Ca}(x; z) + h_K(x; z) + h_{hyp}(x; z) + h_{elec}(x; z) + h_{syn}(x; z)] \quad (1)$$

where  $C_m=1\text{nF}$ , and  $h_{leak}$ ,  $h_{Ca}$ ,  $h_K$ ,  $h_{hyp}$ ,  $h_{elec}$ ,  $h_{syn}$  are the leak, calcium, potassium, hyperpolarization, electrical, and synaptic currents, all of which have their own complicated dependence on  $x$  and  $z = [g_{el}, g_{synA}]$  (see Section A.2.1).

Second, we define the emergent property, which as above is network syncing: oscillation of the entire population at an intermediate frequency of our choosing (Figure 1A bottom). Quantifying this phenomenon is straightforward: we define network syncing to be that each neuron’s spiking frequency – denoted  $\omega_{f1}(x)$ ,  $\omega_{f2}(x)$ , etc. – is close to an intermediate frequency of 0.55Hz. Mathematically, we achieve this via constraints on the mean and variance of  $\omega_i(x)$  for each neuron  $i \in \{f1, f2, hub, s1, s2\}$ , and thus:

$$E[T(x)] \triangleq E \begin{bmatrix} \omega_{f1}(x) \\ \vdots \\ (\omega_{f1}(x) - 0.55)^2 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0.55 \\ \vdots \\ 0.025^2 \\ \vdots \end{bmatrix} \triangleq \mu, \quad (2)$$

which completes the quantification of the emergent property.

Third, we perform emergent property inference: we find a distribution over parameter configurations  $z$ , and insist that samples from this distribution produce the emergent property; in other words, they obey the constraints introduced in Equation 14. This distribution will be chosen from a family of probability distributions  $\mathcal{Q} = \{q_\theta(z) : \theta \in \Theta\}$ , defined by a deep generative distribution of the normalizing flow class [16, 17, 18] – neural networks which transform a simple distribution into a suitably complicated distribution (as is needed here). This deep distribution is represented in Figure 1C (and see Methods for more detail). Then, mathematically, we must solve the following optimization program:

$$\begin{aligned} & \underset{q_\theta \in \mathcal{Q}}{\operatorname{argmax}} H(q_\theta(z)) \\ & \text{s.t. } E_{z \sim q_\theta} [E_{x \sim p(x|z)} [T(x)]] = \mu, \end{aligned} \quad (3)$$

where  $T(x), \mu$  are defined as in Equation 14, and  $p(x|z)$  is the intractable distribution of data from the model ( $x$ ), given that model’s parameters  $z$  (we access samples from this distribution by running

the model forward). The purpose of each element in this program is detailed in Figure 1D. Finally, we recognize that many distributions in  $\mathcal{Q}$  will respect the emergent property constraints, so we require a normative principle to select amongst them. This principle is captured in Equation 3 by the primal objective  $H$ . Here we chose Shannon entropy as a means to find parameter distributions with minimal assumptions beyond some chosen structure [32, 33, 19, 34], but we emphasize that the EPI method is unaffected by this choice (but the results of course will depend on the primal objective chosen).

EPI optimizes the weights and biases  $\theta$  of the deep neural network (which induces the probability distribution) by iteratively solving Equation 3. The optimization is complete when the sampled models with parameters  $z \sim q_\theta$  produce activity consistent with the specified emergent property. Such convergence is evaluated with a hypothesis test that the mean of each emergent property statistic is not different than its emergent property value (see Section A.1.2). Equipped with this method, we now prove out the value of EPI by using it to investigate three prominent models in neuroscience, using EPI to produce new insights about these models.

### 3.3 Comprehensive input-responsivity in a nonlinear sensory system

In studies of primary visual cortex (V1), theoretical models with excitatory (E) and inhibitory (I) populations have reproduced a host of experimentally documented phenomena. In particular regimes of excitation and inhibition, these E/I models exhibit the paradoxical effect [4], selective amplification [35], surround suppression [36], and sensory integrative properties [37]. Extending this model using experimental evidence of three genetically-defined classes of inhibitory neurons [38, 39], recent work [23] has investigated a four-population model – excitatory (E), parvalbumin (P), somatostatin (S), and vasointestinal peptide (V) neurons – as shown in Fig. 2A. The dynamical state of this model is the firing rate of each neuron-type population  $x = [x_E, x_P, x_S, x_V]^\top$ , which evolves according to rectified ( $\llbracket \cdot \rrbracket_+$ ) and exponentiated dynamics:

$$\tau \frac{dx}{dt} = -x + [Wx + h]_+^n \quad (4)$$

with effective connectivity weights  $W$  and input  $h$ . In our analysis, we set the time constant  $\tau = 20\text{ms}$  and dynamics coefficient  $n = 2$ . Also, as is fairly standard, we obtain an informative estimate of the effective connectivities between these neuron-types  $W$  in mice by multiplying their probability of connection with their average synaptic strength [40, 41] (see Section A.2.2). Given

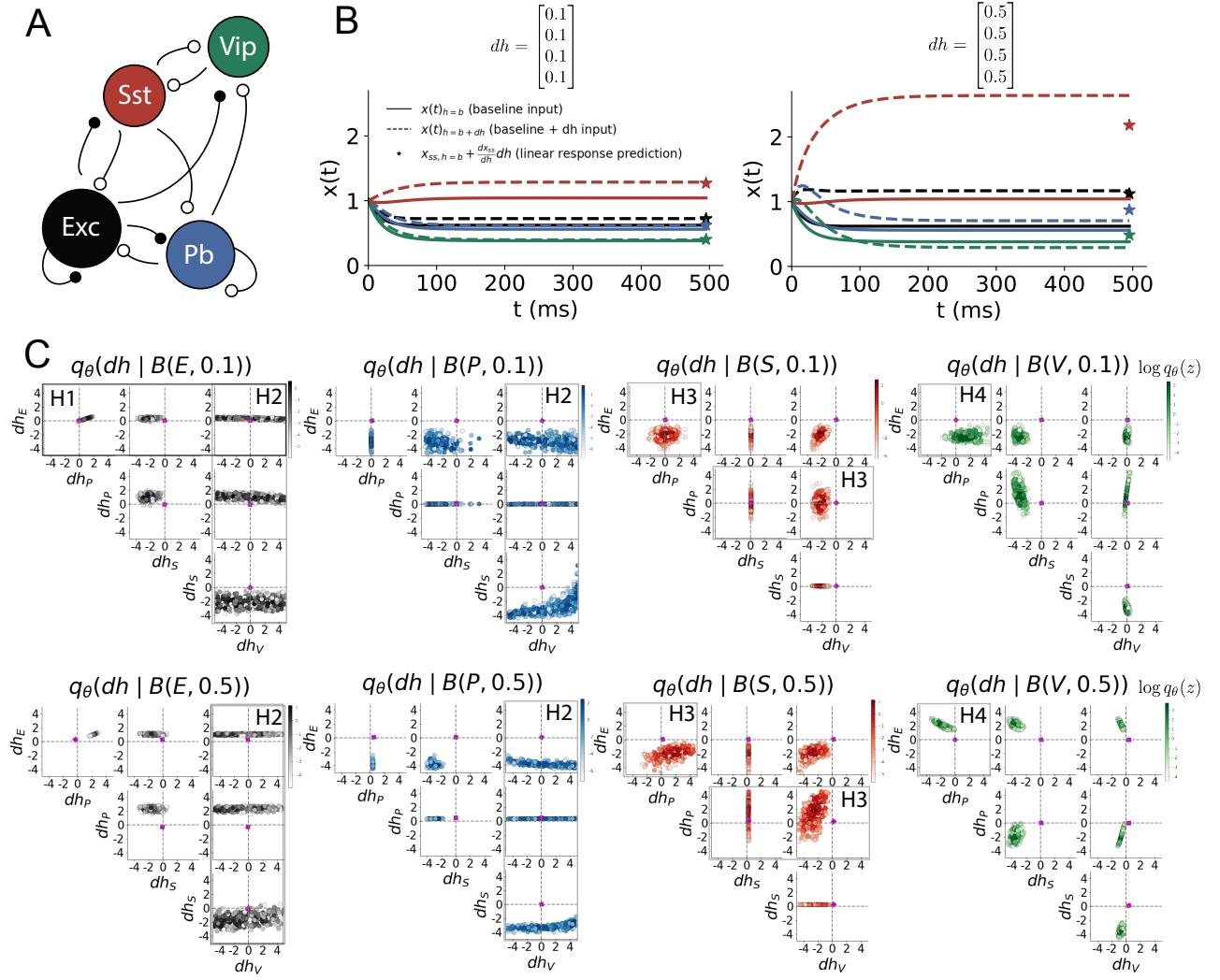


Figure 2: Hypothesis generation through EPI in a V1 model. A. Four-population model of primary visual cortex with excitatory (black), parvalbumin (blue), somatostatin (red), and vip (green) neurons. Some neuron-types largely do not form synaptic projections to others (excitatory and inhibitory projections filled and unfilled, respectively). B. Linear response predictions become inaccurate with greater input strength. V1 model simulations for input ( $b$ ) solid and ( $b + dh$ ) dashed.  $b = [1, 1, 1, 1]^T$  and (left)  $dh = [0.1, 0.1, 0.1, 0.1]^T$  (right)  $dh = [0.5, 0.5, 0.5, 0.5]^T$ . Stars indicate the linear response prediction. C. EPI distributions on differential input  $dh$  conditioned on differential response  $\mathcal{B}(\alpha, y)$ . Supporting evidence for the four generated hypotheses are indicated by gray boxes with labels H1, H2, H3, and H4. The linear prediction from two standard deviations away from  $y$  (from negative to positive) is overlaid in magenta (very small, near origin).

201 these fixed choices of  $W$ ,  $n$ , and  $\tau$ , we studied the system's response to input

$$h = b + dh, \quad (5)$$

202 where the input  $h$  is comprised of a baseline input  $b = [b_E, b_P, b_S, b_V]^\top$  and a differential input  
 203  $dh = [dh_E, dh_P, dh_S, dh_V]^\top$  to each neuron-type population. Throughout subsequent analyses, the  
 204 baseline input is  $b = [1, 1, 1, 1]^\top$ .

205 Having established our model, we now define the emergent property. We begin with the linearized  
 206 response of the system to input  $\frac{dx_{ss}}{dh}$  at the steady state  $x_{ss}$ , i.e. a fixed point. While this lin-  
 207 earization accurately predicts differential responses  $dx_{ss} = [dx_{E,ss}, dx_{P,ss}, dx_{S,ss}, dx_{V,ss}]$  for small  
 208 differential inputs to each population  $dh = [0.1, 0.1, 0.1, 0.1]$  (Fig. 2B, left), linearization is a poor  
 209 predictor in this nonlinear model more generally (Fig. 3B, right). Currently available approaches  
 210 to deriving the steady state response of this system are limited.

211 To get a more comprehensive picture of the input-responsivity of each neuron-type, we used EPI  
 212 to learn a distribution of the differential inputs to each population  $dh$  that produce an increase  
 213 of  $y \in \{0.1, 0.5\}$  in the rate of each neuron-type population  $\alpha \in \{E, P, S, V\}$ . We want to know  
 214 the differential inputs  $dh$  that result in a differential steady state  $dx_{\alpha,ss}$  (the change in  $x_{\alpha,ss}$  when  
 215 receiving input  $h = b + dh$  with respect to the baseline  $h = b$ ) of value  $y$  with some small, arbitrarily  
 216 chosen amount of variance  $0.01^2$ . These statements amount to the emergent property

$$\mathcal{B}(\alpha, y) \triangleq E \begin{bmatrix} dx_{\alpha,ss} \\ (dx_{\alpha,ss} - y)^2 \end{bmatrix} = \begin{bmatrix} y \\ 0.01^2 \end{bmatrix} \quad (6)$$

217 We continue to use  $\mathcal{B}(\cdot)$  throughout the rest of the study as short hand for emergent property, which  
 218 represents a different signature of computation in each application. In Each column of Figure 2C  
 219 visualizes the inferred distribution of  $dh$  corresponding to a excitatory (red), parvalbumin (blue),  
 220 somatostatin (red) and vip (green) neuron-type increase, while each row corresponds to amounts of  
 221 increase 0.1 and 0.5. These distributions conditioned on such emergent properties are now available  
 222 through EPI. For each pair of parameters we show the two-dimensional marginal distribution of  
 223 samples colored by  $\log q_\theta(dh | \mathcal{B}(\alpha, y))$ . The inferred distributions immediately suggest four hy-  
 224 potheses:

225

226 H1: as is intuitive, each neuron-type's firing rate should be sensitive to that neuron-type's direct  
 227 input (e.g. Fig. 2C H1 indicates low variance in  $dh_E$  when  $\alpha = E$ . Same observation in all inferred  
 228 distributions);

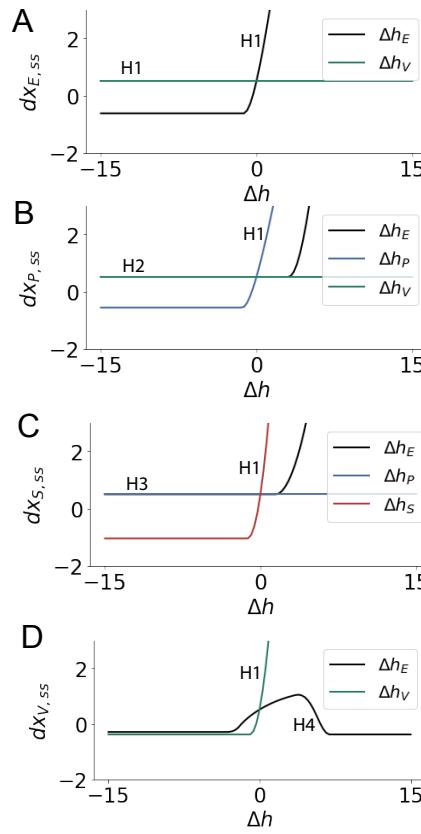


Figure 3: Confirming EPI generated hypotheses in V1. A. Differential responses by the E-population to changes in individual input  $\Delta h_\alpha u_\alpha$  away from the mode of the EPI distribution  $dh^*$ . B-D Same plots for the P-, S-, and V-populations. Labels H1, H2, H3, and H4 indicate which curves confirm which hypotheses.

- 229 H2: the E- and P-populations should be largely unaffected by  $dh_V$  (Fig. 2C H2 indicates high  
230 variance in  $dh_V$  when  $\alpha \in \{E, P\}$ );  
231 H3: the S-population should be largely unaffected by  $dh_P$  (Fig. 2C H3 indicate high variance in  
232  $dh_P$  when  $\alpha = S$ );  
233 H4: there should be a nonmonotonic response of  $dx_{V,ss}$  with  $dh_E$  (Fig. 2C H4 indicates that  
234 negative  $dh_E$  should result in small  $dx_{V,ss}$ , but positive  $dh_E$  should elicit a larger  $dx_{V,ss}$ );  
235 We evaluate these hypotheses by taking steps in individual neuron-type input  $\Delta h_\alpha$  away from the  
236 modes of the inferred distributions at  $y = 0.1$ .

$$dh^* = z^* = \underset{z}{\operatorname{argmax}} \log q_\theta(z | \mathcal{B}(\alpha, 0.1)) \quad (7)$$

- 237 Now,  $dx_{\alpha,ss}$  is the steady state response to the system with input  $h = b + dh^* + \Delta h_\alpha u_\alpha$  where  $u_\alpha$   
238 is a unit vector in the dimension of  $\alpha$ . The EPI-generated hypotheses are confirmed.

- 239 • the neuron-type responses are sensitive to their direct inputs (Fig. 3A black, 3B blue, 3C  
240 red, 3D green);  
241 • the E- and P-populations are not affected by  $dh_V$  (Fig. 3A green, 3B green);

- 242     • the S-population is not affected by  $dh_P$  (Fig. 3C blue);  
 243     • the V-population exhibits a nonmonotonic response to  $dh_E$  (Fig. 3D black), and is in fact  
 244       the on population to do so (Fig. 3A-C black).

245 These hypotheses were in stark contrast to what was available to us via traditional analytical linear  
 246 prediction (Fig. 2C, magenta). To this point, we have shown the utility of EPI on relatively low-  
 247 level emergent properties like network syncing and differential neuron-type population responses.  
 248 In the remainder of the study, we focus on using EPI to understand models of more abstract  
 249 cognitive function.

250 **3.4 Identifying neural mechanisms of behavioral learning.**

251 Identifying measurable biological changes that result in improved behavior is important for neuro-  
 252 science, since they may indicate how the learning brain adapts. In a rapid task switching experiment  
 253 [42], rats were explicitly cued on each trial to either orient towards a visual stimulus in the Pro  
 254 (P) task or orient away from a visual stimulus in the Anti (A) task (Fig. 3a). Neural recordings  
 255 in the midbrain superior colliculus (SC) exhibited two populations of neurons that simultaneously  
 256 represented both task context (Pro or Anti) and motor response (contralateral or ipsilateral to the  
 257 recorded side): the Pro/Contra and Anti/Ipsi neurons [24]. Duan et al. proposed a model of SC  
 258 that, like the V1 model analyzed in the previous section, is a four-population dynamical system.  
 259 Here, the neuron-type populations are functionally-defined as the Pro- and Anti-populations in each  
 260 hemisphere (left (L) and right (R)). The Pro- or Anti-populations receive an input determined by  
 261 the cue, and then the left and right populations receive an input based on the side of the light  
 262 stimulus. Activities were bounded between 0 and 1, so that a high output of the Pro population  
 263 in a given hemisphere corresponds to the contralateral response. An additional stipulation is that  
 264 when one Pro population responds with a high-output, the opposite Pro population must respond  
 265 with a low output. Finally, this circuit operates in the presence of Gaussian noise resulting in trial-  
 266 to-trial variability (see Section A.2.3). The connectivity matrix is parameterized by the geometry  
 267 of the population arrangement (Fig. 3B).

268 Here, we used EPI to learn distributions of the SC weight matrix parameters  $z = W$  conditioned  
 269 on various levels of rapid task switching accuracy  $\mathcal{B}(p)$  for  $p \in \{50\%, 60\%, 70\%, 80\%, 90\%\}$  (see  
 270 Section A.2.3). Following the approach in Duan et al., we decomposed the connectivity matrix  
 271  $W = QAQ^{-1}$  in such a way (the Schur decomposition) that the basis vectors  $q_i$  are the same for all

<sup>272</sup>  $W$  (Fig. 3C). These basis vectors have intuitive roles in processing for this task, and are accordingly  
<sup>273</sup> named the *all* mode - all neurons co-fluctuate, *side* mode - one side dominates the other, *task* mode  
<sup>274</sup> - the Pro or Anti populations dominate the other, and *diag* mode - Pro- and Anti-populations of  
<sup>275</sup> opposite hemispheres dominate the opposite pair. The corresponding eigenvalues (e.g.  $a_{\text{task}}$ , which  
<sup>276</sup> change according to  $W$ ) indicate the degree to which activity along that mode is increased or  
<sup>277</sup> decreased by  $W$ .

<sup>278</sup> EPI demonstrates that, for greater task accuracies, the task mode eigenvalue increases, indicating  
<sup>279</sup> the importance of  $W$  to the task representation (Fig. 4D, purple). Stepping from random chance  
<sup>280</sup> (50%) networks to marginally task-performing (60%) networks, there is a marked decrease of the  
<sup>281</sup> side mode eigenvalues (Fig. 3D, orange). Such side mode suppression remains in the models  
<sup>282</sup> achieving greater accuracy, revealing its importance towards task performance. There were no  
<sup>283</sup> interesting trends with learning in the all or diag mode (hence not shown in Fig. 3). Importantly,  
<sup>284</sup> we can conclude from our methodology that side mode suppression in  $W$  allows rapid task switching,  
<sup>285</sup> and that greater task-mode representations in  $W$  increase accuracy. These hypotheses are confirmed  
<sup>286</sup> by forward simulation of the SC model (Fig. 3E). Thus, EPI produces novel, experimentally testable  
<sup>287</sup> predictions: effective connectivity between these populations changes throughout learning, in a way  
<sup>288</sup> that increases its task mode and decreases its side mode eigenvalues.

### <sup>289</sup> 3.5 Linking RNN connectivity to computational error

<sup>290</sup> So far, each model we have studied was designed from fundamental biophysical principles, genetically-  
<sup>291</sup> or functionally-defined neuron types. At a more abstract level of modeling, recurrent neural net-  
<sup>292</sup> works (RNNs) are high-dimensional dynamical models of computation that are becoming increas-  
<sup>293</sup> ingly popular in neuroscience research [43]. In theoretical neuroscience, RNN dynamics usually  
<sup>294</sup> follow the equation

$$\frac{dx}{dt} = -x(t) + W\phi(x(t)) + I(t), \quad (8)$$

<sup>295</sup> where  $x(t)$  is the network activity,  $W$  is the network connectivity,  $\phi(\cdot) = \tanh(\cdot)$ , and  $I(t)$  is the  
<sup>296</sup> input to the system. Such RNNs are trained to do a task from a systems neuroscience experiment,  
<sup>297</sup> and then the unit activations of the trained RNN are compared to recorded neural activity. Fully-  
<sup>298</sup> connected RNNs with tens of thousands of parameters are challenging to characterize [44], especially  
<sup>299</sup> making statistical inferences about their parameterization. Alternatively, we consider a rank-1,  $N$ -  
<sup>300</sup> neuron RNN with connectivity

$$W = g\chi + \frac{1}{N}mn^\top, \quad (9)$$

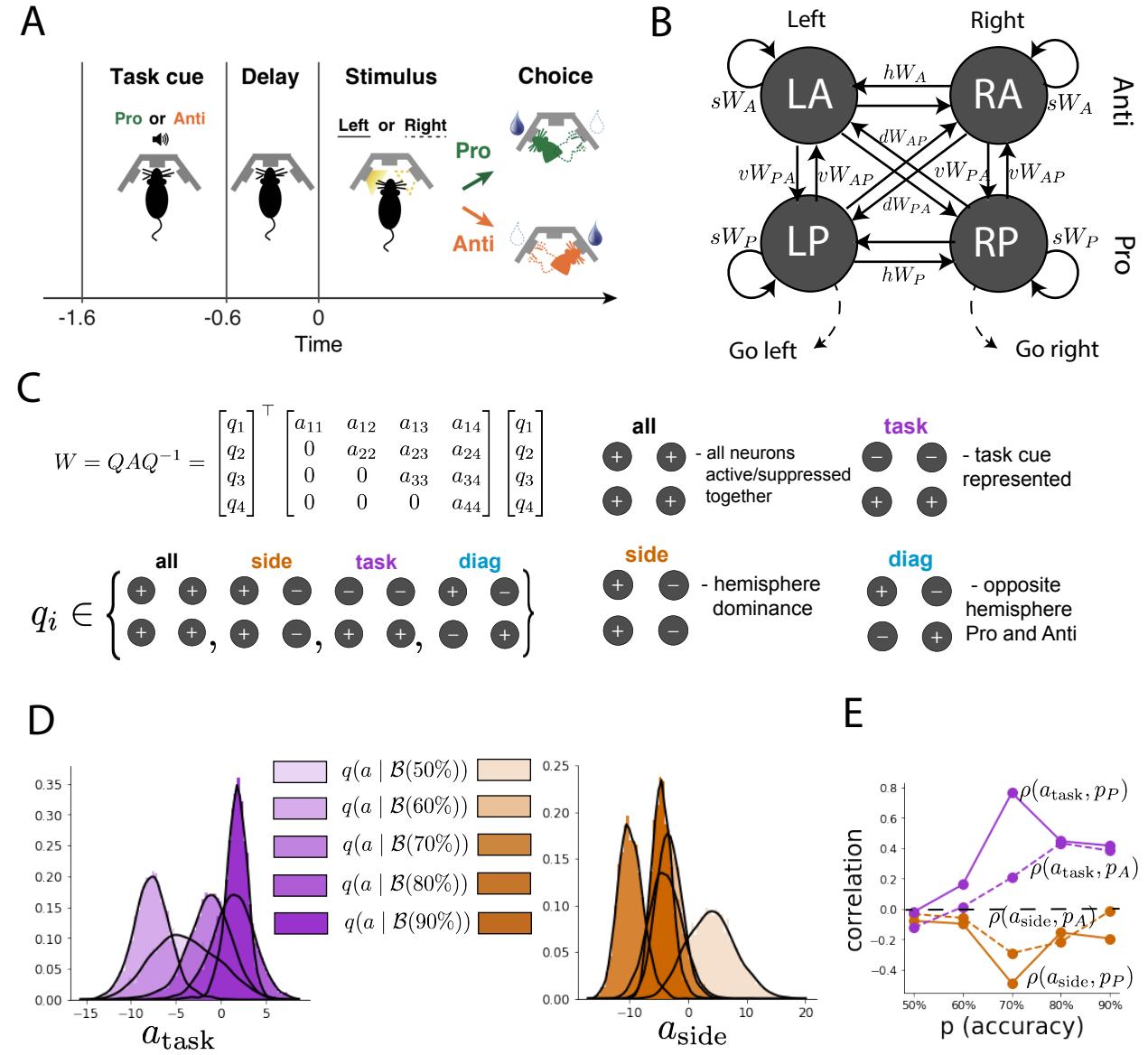


Figure 4: EPI reveals changes in SC [24] connectivity that control task accuracy. A. Rapid task switching behavioral paradigm (see text). B. Model of superior colliculus (SC). Neurons: LP - left pro, RP - right pro, LA - left anti, RA - right anti. Parameters:  $sW$  - self,  $hW$  - horizontal,  $vW$  - vertical,  $dW$  - diagonal weights. C. The Schur decomposition of the weight matrix  $W = QAQ^{-1}$  is a unique decomposition with orthogonal  $Q$  and upper triangular  $A$ . Schur modes:  $q_{all}$ ,  $q_{task}$ ,  $q_{side}$ , and  $q_{diag}$ . D. The marginal EPI distributions of the Schur eigenvalues at each level of task accuracy. E. The correlation of Schur eigenvalue with task performance in each learned EPI distribution.

301 where  $\chi_{ij} \sim \mathcal{N}(0, \frac{1}{N})$ ,  $g$  is the random strength, and the entries of  $m$  and  $n$  are drawn from Gaussian  
 302 distributions  $m_i \sim \mathcal{N}(M_m, 1)$  and  $n_i \sim \mathcal{N}(M_n, 1)$ . We use EPI to infer the parameterizations of  
 303 rank-1 RNNs solving an example task, enabling discovery of properties of connectivity that result  
 304 in different types of computational errors.

305 The task we consider is Gaussian posterior conditioning: calculate the parameters of a posterior  
 306 distribution induced by a prior  $p(\mu_y) = \mathcal{N}(\mu_0 = 4, \sigma_0^2 = 1)$  and a likelihood  $p(y|\mu_y) = \mathcal{N}(\mu_y, \sigma_y^2 =$   
 307  $1)$ , given a single observation  $y$ . Conjugacy offers the result analytically;  $p(\mu_y|y) = \mathcal{N}(\mu_{post}, \sigma_{post}^2)$ ,  
 308 where:

$$\mu_{post} = \frac{\frac{\mu_0}{\sigma_0^2} + \frac{y}{\sigma_y^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma_y^2}} \quad \sigma_{post}^2 = \frac{1}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma_y^2}}. \quad (10)$$

309 The RNN is trained to solve this task by producing readout activity that is on average the posterior  
 310 mean  $\mu_{post}$ , and activity whose variability is the posterior variance  $\sigma_{post}^2$  (a setup inspired by  
 311 [45]). To solve this Gaussian posterior conditioning task, the RNN response to a constant input  
 312  $I(t) = yw + (n - M_n)$  must equal the posterior mean along readout vector  $w$ , where

$$\kappa_w = \frac{1}{N} \sum_{j=1}^N w_j \phi(x_j) \quad (11)$$

313 Additionally, the amount of chaotic variance  $\Delta_T$  must equal the posterior variance.  $\kappa_w$  and  $\Delta_T$  can  
 314 be expressed in terms of each other through a solvable system of nonlinear equations (see Section  
 315 A.2.4) [25]. This theory allows us to mathematically formalize the execution of this task into an  
 316 emergent property, where the emergent property statistics of the RNN activity are  $k_w$  and  $\Delta_T$  and  
 317 the emergent property values are the ground truth posterior mean  $\mu_{post}$  and variance  $\sigma_{post}^2$ :

$$E \begin{bmatrix} \kappa_w \\ \Delta_T \\ (\kappa_w - \mu_{post})^2 \\ (\Delta_T^2 - \sigma_{post}^2)^2 \end{bmatrix} = \begin{bmatrix} \mu_{post} \\ \sigma_{post}^2 \\ 0.1 \\ 0.1 \end{bmatrix} \quad (12)$$

318 We specify a substantial amount of variability in the variance constraints so that the inferred  
 319 distribution results in RNNs with a variety biases in their solutions to the gaussian posterior  
 320 conditioning problem.

321 We used EPI to learn distributions of RNN connectivity properties  $z = [g \ M_m \ M_n]$  executing  
 322 Gaussian posterior conditioning given an input of  $y = 2$ . (see Section A.2.4) (Fig. 5B). The true  
 323 Gaussian conditioning posterior for an input of  $y = 2$  is  $\mu_{post} = 3$  and  $\sigma_{post} = 0.5$ . We examined  
 324 the nature of the over- and under-estimation of the posterior means (Fig. 5B, left) and variances

(Fig. 5B, right) in the inferred distributions. There is rough symmetry in the  $M_m$ - $M_n$  plane, suggesting a degeneracy in the product of  $M_m$  and  $M_n$  (Fig. 5B). The product of  $M_m$  and  $M_n$  almost completely determines the posterior mean (Fig. 5B, left), and the random strength  $g$  is the most influential variable on the temporal variance (Fig. 5B, right). Neither of these observations were obvious from what mathematical analysis is available in networks of this type (see Section A.2.4). They lead to the following hypotheses:

H1: The posterior mean of the RNN increases with the product of  $M_m$  and  $M_n$ ;

H2: The posterior variance increases with  $g$ ;

Testing these now in finite-size networks. Will write end of this later.

This novel procedure of doing inference in interpretable parameterizations of RNNs conditioned on the emergent property of task execution is straightforwardly generalizable to other tasks like noisy integration and context-dependent decision making (Fig. S1).

## 4 Discussion

### 4.1 EPI is a general tool for theoretical neuroscience

Models of biological systems are often comprised of complex nonlinear differential equations, making traditional theoretical analysis and statistical inference intractable. In contrast, EPI is capable of learning distributions of parameters in such models producing measurable signatures of computation. We have demonstrated its utility on biological models (STG), intermediate-level models of interacting genetically- and functionally-defined neuron-types (V1, SC), and the most abstract of models (RNNs). We are able to condition both deterministic and stochastic models on low-level emergent properties like firing rates of membrane potentials, as well as high-level cognitive function like Gaussian posterior conditioning. Technically, EPI is tractable when the emergent property statistics are continuously differentiable with respect to the model parameters, which is very often the case; this emphasizes the general utility of EPI.

In this study, we have focused on applying EPI to low dimensional parameter spaces of models with low dimensional dynamical state. These choices were made to present the reader with a series of interpretable conclusions, which is more challenging in high dimensional spaces. In fact, EPI should scale reasonably to high dimensional parameter spaces, as the underlying technology has

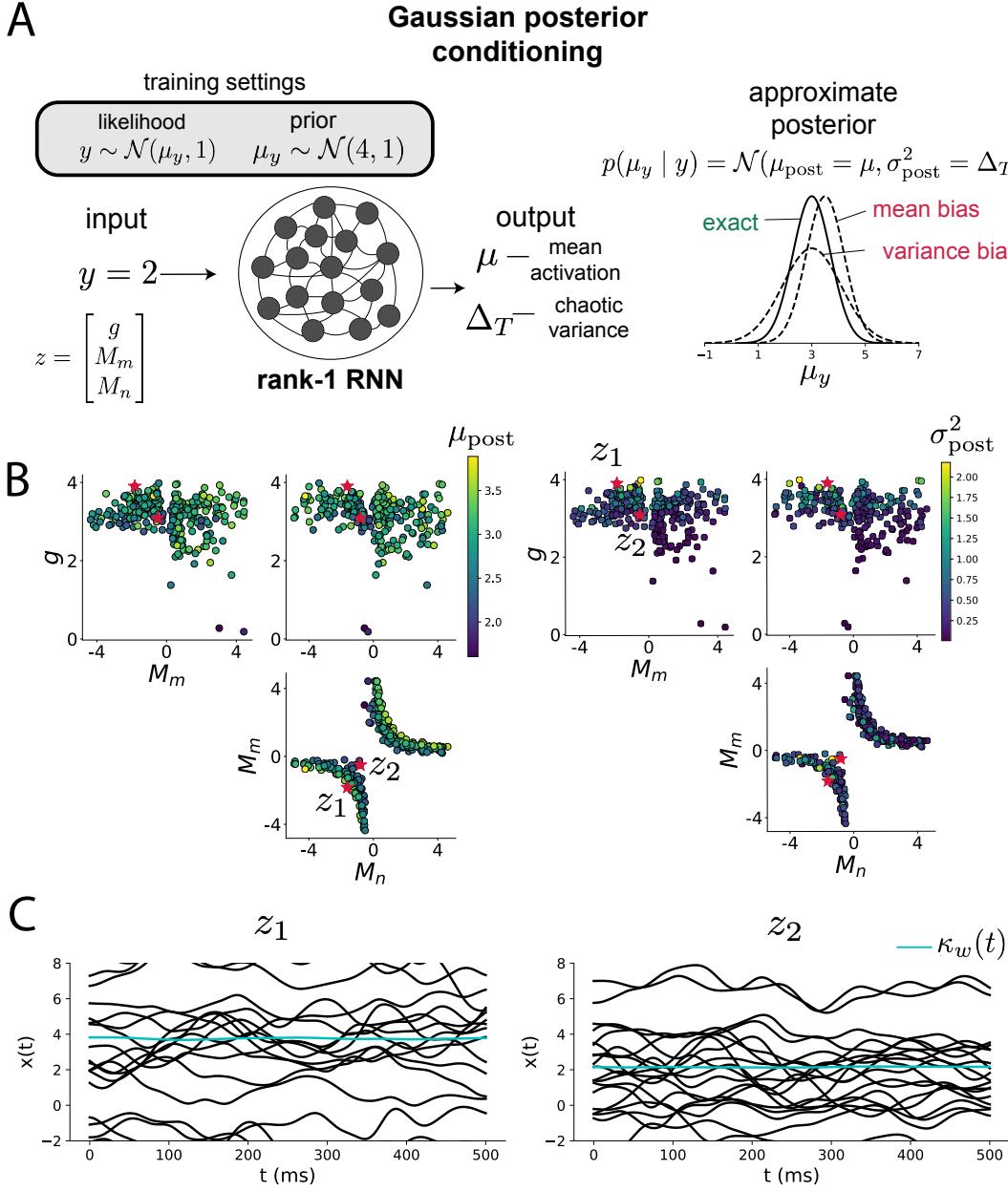


Figure 5: Sources of solution bias in an RNN computation. A. (left) A rank-1 RNN executing a Gaussian posterior conditioning computation on  $\mu_y$ . (right) Bias in this computation can come from over- or under-estimating the posterior mean or variance. B. EPI distribution of rank-1 RNNs executing Gaussian posterior conditioning. Samples are colored by (left) posterior mean  $\mu_{\text{post}} = \kappa_w$  and (right) posterior variance  $\sigma_{\text{post}}^2 = \Delta_T$ . C. Finite-size networks sampled from the distribution perform the calculation and have the computational biases expected from their parameter values. Activity along readout  $\kappa_w$  (cyan).

354 produced state-of-the-art performance on high-dimensional tasks such as texture generation [19].  
 355 Of course, increasing the dimensionality of the dynamical state of the model makes optimization  
 356 more expensive, and there is a practical limit there as with any machine learning approach. For  
 357 systems with high dimensional state, we recommend using theoretical approaches (e.g. [25]) to  
 358 reason about reduced parameterizations of such high-dimensional systems.

359 There are additional technical considerations when assessing the suitability of EPI for a particu-  
 360 lar modeling question. First and foremost, as in any optimization problem, the defined emergent  
 361 property should always be appropriately conditioned (constraints should not have wildly different  
 362 units). Furthermore, if the program is underconstrained (not enough constraints), the distribution  
 363 grows (in entropy) unstably unless mapped to a finite support. If overconstrained, there is no pa-  
 364 rameter set producing the emergent property, and EPI optimization will fail (appropriately). Next,  
 365 one should consider the computational cost of the gradient calculations. In the best circumstance,  
 366 there is a simple, closed form expression (e.g. Section A.1.1) for the emergent property statistic  
 367 given the model parameters. On the other end of the spectrum, many forward simulation iterations  
 368 may be required before a high quality measurement of the emergent property statistic is available  
 369 (e.g. Section A.2.1). In such cases, optimization will be expensive.

370 **4.2 Novel hypotheses from EPI**

371 Machine learning has played an effective, multifaceted role in neuroscientific progress. Primarily,  
 372 it has revealed structure in large-scale neural datasets [46, 47, 48, 49, 50, 51] (see review, [14]).  
 373 Secondarily, trained algorithms of varying degrees of biological relevance are beginning to be viewed  
 374 as fully-observable computational systems comparable to the brain [44, 52].

375 For example, consider the fact that we do not fully understand the four-dimensional models of V1  
 376 [23]. Because analytical approaches to studying nonlinear dynamical systems become increasingly  
 377 complicated when stepping from two-dimensional to three- or four-dimensional systems in the  
 378 absence of restrictive simplifying assumptions [53], it is unsurprising that this model has been a  
 379 challenge. In Section 3.3, we showed that EPI was far more informative about neuron-type input  
 380 responsibility than the predictions afforded through analysis. By flexibly conditioning this V1 model  
 381 on different emergent properties, we performed an exploratory analysis of a *model* rather than a  
 382 dataset, which generated and proved out a set of testable predictions.

383 Of course, exploratory analyses can also be directed. For example, when interested in model

384 changes during learning, one can use EPI to condition as we did in Section 3.4. This analysis  
385 identified experimentally testable predictions (proved out *in-silico*) of changes in connectivity in  
386 SC throughout learning. Precisely, we predict that an initial reduction in side mode eigenvalue,  
387 and a steady increase in task mode eigenvalue will take place, during learning, in the effective  
388 connectivity matrices of learning rats.

389 In our final analysis, we present a novel procedure for doing statistical inference on interpretable  
390 parameterizations of RNNs executing simple tasks . This methodology relies on recently extended  
391 theory of responses in random neural networks with minimal structure [25]. With this methodology,  
392 we can finally open the probabilistic model selection toolkit reasoning about the connectivity of  
393 RNNs solving tasks.

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542 **A Methods**

543 **A.1 Emergent property inference (EPI)**

544 Emergent property inference (EPI) learns distributions of theoretical model parameters that pro-  
 545 duce emergent properties of interest. EPI combines ideas from likelihood-free variational inference  
 546 [20] and maximum entropy flow networks [19]. A maximum entropy flow network is used as a deep  
 547 probability distribution for the parameters, while these samples often parameterize a differentiable  
 548 model simulator, which may lack a tractable likelihood function.

549 Consider model parameterization  $z$  and data  $x$  generated from some theoretical model simulator  
 550 represented as  $p(x | z)$ , which may be deterministic or stochastic. Theoretical models usually have  
 551 known sampling procedures for simulating activity given a circuit parameterization, yet often lack  
 552 an explicit likelihood function due to the nonlinearities and dynamics. With EPI, a distribution  
 553 on parameters  $z$  is learned, that yields an emergent property of interest  $\mathcal{B}$ ,

$$\mathcal{B} \leftrightarrow E_{z \sim q_\theta} [E_{x \sim p(x|z)} [T(x)]] = \mu \quad (13)$$

554 by making an approximation  $q_\theta(z)$  to  $p(z | \mathcal{B})$  (see Section A.1.5). So, over the DSN distribution  
 555  $q_\theta(z)$  of model  $p(x | z)$  for behavior  $\mathcal{B}$ , the emergent properties  $T(x)$  are constrained in expectation  
 556 to  $\mu$ .

557 In deep probability distributions, a simple random variable  $w \sim p_0$  is mapped deterministically  
 558 via a function  $f_\theta$  parameterized by a neural network to the support of the distribution of interest  
 559 where  $z = f_\theta(w) = f_l(\dots f_1(w))$ . Given a theoretical model  $p(x | z)$  and some behavior of interest  
 560  $\mathcal{B}$ , the deep probability distributions are trained by optimizing the neural network parameters  $\theta$  to  
 561 find a good approximation  $q_\theta^*$  within the deep variational family  $Q$  to  $p(z | \mathcal{B})$ .

562 In most settings (especially those relevant to theoretical neuroscience) the likelihood of the behavior  
 563 with respect to the model parameters  $p(T(x) | z)$  is unknown or intractable, requiring an alternative  
 564 to stochastic gradient variational Bayes [5] or black box variational inference[54]. These types  
 565 of methods called likelihood-free variational inference (LFVI, [20]) skate around the intractable  
 566 likelihood function in situations where there is a differentiable simulator. Akin to LFVI, DSNs are  
 567 optimized with the following objective for a given theoretical model, emergent property statistics  
 568  $T(x)$ , and emergent property constraints  $\mu$ :

$$\begin{aligned} q_\theta^*(z) &= \operatorname{argmax}_{q_\theta \in Q} H(q_\theta(z)) \\ \text{s.t. } E_{z \sim q_\theta} [E_{x \sim p(x|z)} [T(x)]] &= \mu \end{aligned} \quad (14)$$

569 Optimizing this objective is a technological accomplishment in its own right, the details of which  
 570 we elaborate in Section A.1.2. Before going through those details, we ground this optimization in  
 571 a toy example.

572 **A.1.1 Example: 2D LDS**

573 To gain intuition for EPI, consider two-dimensional linear dynamical systems,  $\tau \dot{x} = Ax$  with

$$A = \begin{bmatrix} a_1 & a_2 \\ a_3 & a_4 \end{bmatrix}$$

574 that produce a band of oscillations. To do EPI with the dynamics matrix elements as the free  
 575 parameters  $z = [a_1, a_2, a_3, a_4]$ , and fixing  $\tau = 1$ , such that the posterior yields a band of oscillations,  
 576 the emergent property statistics  $T(x)$  are chosen to contain the first- and second-moments of the  
 577 oscillatory frequency  $\Omega$  and the growth/decay factor  $d$  of the oscillating system. To learn the  
 578 distribution of real entries of  $A$  that yield a distribution of  $d$  with mean zero with variance  $0.25^2$ ,  
 579 and oscillation frequency  $\Omega$  with mean 1 Hz with variance  $(0.1\text{Hz})^2$ , then we would select the real  
 580 part of the complex conjugate eigenvalues  $\text{real}(\lambda_1) = d$  (via an arbitrary choice of eigenvalue of the  
 581 dynamics matrix  $\lambda_1$ ) and the positive imaginary component of one of the eigenvalues  $\text{imag}(\lambda_1) =$   
 582  $2\pi\Omega$  as the emergent property statistics. Those emergent property statistics are then constrained  
 583 to

$$\mu = E \begin{bmatrix} \text{real}(\lambda_1) \\ \text{imag}(\lambda_1) \\ (\text{real}(\lambda_1) - 0)^2 \\ (\text{imag}(\lambda_1) - 2\pi\Omega)^2 \end{bmatrix} = \begin{bmatrix} 0.0 \\ 2\pi\Omega \\ 0.25^2 \\ (2\pi 0.1)^2 \end{bmatrix} \quad (15)$$

584 where  $\Omega = 1\text{Hz}$ . Unlike the models we study in the paper which calculate  $E_{x \sim p(x|z)} [T(x)]$  via  
 585 forward simulation, we have a closed form for the eigenvalues of the dynamics matrix.  $\lambda$  can be  
 586 calculated using the quadratic formula:

$$\lambda = \frac{\left(\frac{a_1+a_4}{\tau}\right) \pm \sqrt{\left(\frac{a_1+a_4}{\tau}\right)^2 + 4\left(\frac{a_2a_3-a_1a_4}{\tau}\right)}}{2} \quad (16)$$

587 where  $\lambda_1$  is the eigenvalue of  $\frac{1}{\tau}A$  with greatest real part. Even though  $E_{x \sim p(x|z)} [T(x)]$  is calculable  
 588 directly via a closed form function and does not require simulation, we cannot derive the distribution  
 589  $q_\theta^*$  directly. This is due to the formally hard problem of the backward mapping: finding the natural  
 590 parameters  $\eta$  from the mean parameters  $\mu$  of an exponential family distribution [55]. Instead, we  
 591 can use EPI to learn the linear system parameters producing such a band of oscillations (Fig. S2B).

592 Even this relatively simple system has nontrivial (though intuitively sensible) structure in the  
 593 parameter distribution. To validate our method (further than that of the underlying technology  
 594 on a ground truth solution [19]) we can analytically derive the contours of the probability density



Fig. S2: A. Two-dimensional linear dynamical system model, where real entries of the dynamics matrix  $A$  are the parameters. B. The DSN distribution for a 2D LDS with  $\tau = 1$  that produces an average of 1Hz oscillations with some small amount of variance. C. Entropy throughout the optimization. At the beginning of each augmented Lagrangian epoch (5,000 iterations), the entropy dips due to the shifted optimization manifold where emergent property constraint satisfaction is increasingly weighted. D. Emergent property moments throughout optimization. At the beginning of each augmented Lagrangian epoch, the emergent property moments move closer to their constraints.

595 from the emergent property statistics and values (Fig. S3). In the  $a_1 - a_4$  plane, is a black line  
 596 at  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} = 0$ , a dotted black line at the standard deviation  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} \pm 1$ , and a  
 597 grey line at twice the standard deviation  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} \pm 2$  (Fig. S3A). Here the lines denote the  
 598 set of solutions at fixed behaviors, which overlay the posterior obtained through EPI. The learned  
 599 DSN distribution precisely reflects the desired statistical constraints and model degeneracy in the  
 600 sum of  $a_1$  and  $a_4$ . Intuitively, the parameters equivalent with respect to emergent property statistic  
 601  $\text{real}(\lambda_1)$  have similar log densities.

602 To explain the structure in the bimodality of the DSN posterior, we can look at the imaginary  
 603 component of  $\lambda_1$ . When  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} = 0$ , we have

$$\text{imag}(\lambda_1) = \begin{cases} \sqrt{\frac{a_1a_4-a_2a_3}{\tau}}, & \text{if } a_1a_4 < a_2a_3 \\ 0 & \text{otherwise} \end{cases} \quad (17)$$

604 When  $\tau = 1$  and  $a_1a_4 > a_2a_3$  (center of distribution above), we have the following equation for the  
 605 other two dimensions:

$$\text{imag}(\lambda_1)^2 = a_1a_4 - a_2a_3 \quad (18)$$

606 Since we constrained  $E_{q_\theta}[\text{imag}(\lambda)] = 2\pi$  (with  $\omega = 1$ ), we can plot contours of the equation  
 607  $\text{imag}(\lambda_1)^2 = a_1a_4 - a_2a_3 = (2\pi)^2$  for various  $a_1a_4$  (Fig. S3A). If  $\sigma_{1,4} = E_{q_\theta}(|a_1a_4 - E_{q_\theta}[a_1a_4]|)$ ,  
 608 then we plot the contours as  $a_1a_4 = 0$  (black),  $a_1a_4 = -\sigma_{1,4}$  (black dotted), and  $a_1a_4 = -2\sigma_{1,4}$   
 609 (grey dotted) (Fig. S3B). This validates the curved structure of the inferred distribution learned  
 610 through EPI. We take steps in negative standard deviation of  $a_1a_4$  (dotted and gray lines), since  
 611 there are few positive values  $a_1a_4$  in the posterior. Subtler model-behavior combinations will have  
 612 even more complexity, further motivating the use of EPI for understanding these systems. Indeed,  
 613 we sample a distribution of systems oscillating near 1Hz (Fig. S4).

### 614 A.1.2 Augmented Lagrangian optimization

615 To optimize  $q_\theta(z)$  in Equation ??, the constrained optimization is performed using the augmented  
 616 Lagrangian method. The following objective is minimized:

$$L(\theta; \alpha, c) = -H(q_\theta) + \alpha^\top \delta(\theta) + \frac{c}{2} \|\delta(\theta)\|^2 \quad (19)$$

617 where  $\delta(\theta) = E_{z \sim q_\theta} [E_{x \sim p(x|z)} [T(x) - \mu]]$ ,  $\alpha \in \mathcal{R}^m$  are the Lagrange multipliers and  $c$  is the penalty  
 618 coefficient. For a fixed  $(\alpha, c)$ ,  $\theta$  is optimized with stochastic gradient descent. A low value of  $c$  is

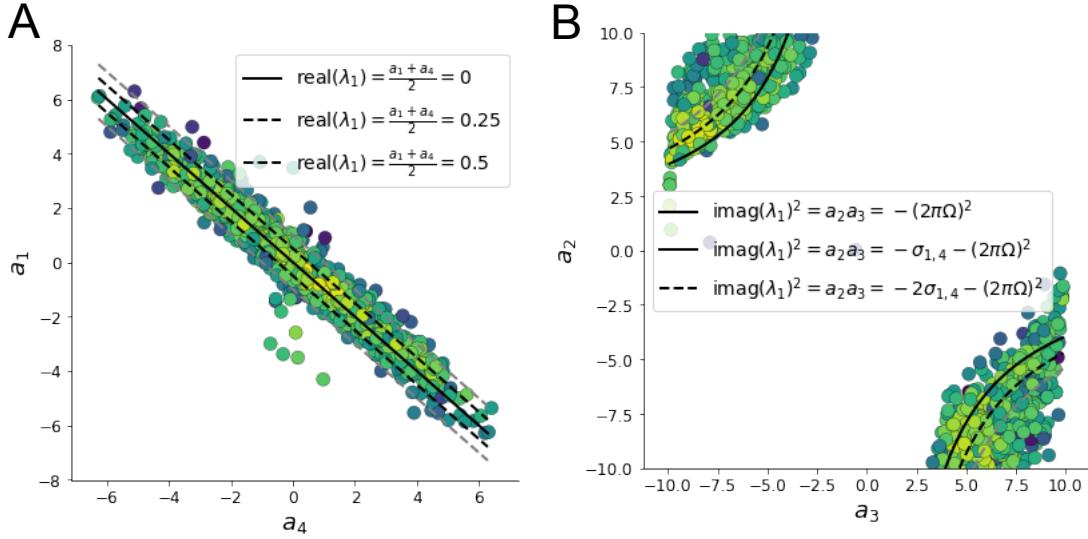


Fig. S3: A. Probability contours in the  $a_1 - a_4$  plane can be derived from the relationship to emergent property statistic of growth/decay factor. B. Probability contours in the  $a_2 - a_3$  plane can be derived from relationship to the emergent property statistic of oscillation frequency.

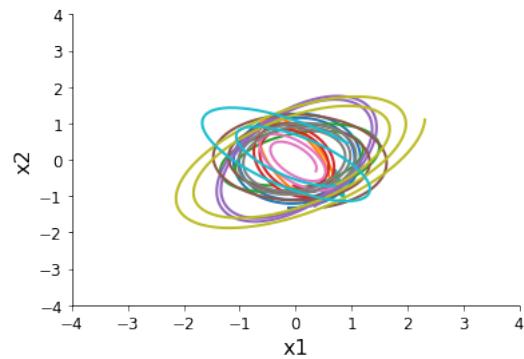


Fig. S4: Sampled dynamical system trajectories from the EPI distribution. Each trajectory is initialized at  $x(0) = \left[ \frac{\sqrt{2}}{2} \quad -\frac{\sqrt{2}}{2} \right]$ .

used initially, and increased during each augmented Lagrangian epoch – a period of optimization with fixed  $\alpha$  and  $c$  for a given number of stochastic optimization iterations. Similarly,  $\alpha$  is tuned each epoch based on the constraint violations. For the linear 2-dimensional system (Fig. S2C) optimization hyperparameters are initialized to  $c_1 = 10^{-4}$  and  $\alpha_1 = 0$ . The penalty coefficient is updated based on a hypothesis test regarding the reduction in constraint violation. The p-value of  $E[|\delta(\theta_{k+1})|] > \gamma E[|\delta(\theta_k)|]$  is computed, and  $c_{k+1}$  is updated to  $\beta c_k$  with probability  $1 - p$ . Throughout the project,  $\beta = 4.0$  and  $\gamma = 0.25$  is used. The other update rule is  $\alpha_{k+1} = \alpha_k + c_k \frac{1}{n} \sum_{i=1}^n (T(x^{(i)}) - \mu)$ . In this example, each augmented Lagrangian epoch ran for 2,000 iterations. We consider the optimization to have converged when a null hypothesis test of constraint violations being zero is accepted for all constraints at a significance threshold 0.05. This is the dotted line on the plots below depicting the optimization cutoff of EPI optimization for the 2-dimensional linear system. If the optimization is left to continue running, entropy usually decreases, and structural pathologies in the distribution may be introduced.

The intention is that  $c$  and  $\alpha$  start at values encouraging entropic growth early in optimization. Then, as they increase in magnitude with each training epoch, the constraint satisfaction terms are increasingly weighted, resulting in a decrease in entropy. Rather than using a naive initialization, before EPI, we optimize the deep probability distribution parameters to generate samples of an isotropic Gaussian of a selected variance, such as 1.0 for the 2D LDS example. This provides a convenient starting point, whose level of entropy is controlled by the user.

### 638 A.1.3 Normalizing flows

Since we are optimizing parameters  $\theta$  of our deep probability distribution with respect to the entropy, we will need to take gradients with respect to the log-density of samples from the deep probability distribution.

$$H(q_\theta(z)) = \int -q_\theta(z) \log(q_\theta(z)) dz = E_{z \sim q_\theta} [-\log(q_\theta(z))] = E_{\omega \sim q_0} [-\log(q_\theta(f_\theta(\omega)))] \quad (20)$$

$$\nabla_\theta H(q_\theta(z)) = E_{\omega \sim q_0} [-\nabla_\theta \log(q_\theta(f_\theta(\omega)))] \quad (21)$$

Deep probability models typically consist of several layers of fully connected neural networks. When each neural network layer is restricted to be a bijective function, the sample density can be calculated using the change of variables formula at each layer of the network. For  $z' = f(z)$ ,

$$q(z') = q(f^{-1}(z')) \left| \det \frac{\partial f^{-1}(z')}{\partial z'} \right| = q(z) \left| \det \frac{\partial f(z)}{\partial z} \right|^{-1} \quad (22)$$

646 However, this computation has cubic complexity in dimensionality for fully connected layers. By  
 647 restricting our layers to normalizing flows [16] – bijective functions with fast log determinant ja-  
 648 cobian computations, we can tractably optimize deep generative models with objectives that are a  
 649 function of sample density, like entropy. Most of our analyses use real NVP [56], which have proven  
 650 effective in our architecture searches, and have the advantageous features of fast sampling and fast  
 651 density evaluation.

652 **A.1.4 Related work**

653 (To come)

654

655 **A.1.5 Emergent property inference as variational inference in an exponential family**

656 (To come)

657

658 **A.2 Theoretical models**

659 In this study, we used emergent property inference to examine several models relevant to theoretical  
 660 neuroscience. Here, we provide the details of each model and the related analyses.

661 **A.2.1 Stomatogastric ganglion**

662 Each neuron's membrane potential  $x_m(t)$  is the solution of the following differential equation.

$$C_m \frac{dx_m}{dt} = -[h_{leak}(x; z) + h_{Ca}(x; z) + h_K(x; z) + h_{hyp}(x; z) + h_{elec}(x; z) + h_{syn}(x; z)] \quad (23)$$

663 The membrane potential of each neuron is affected by the leak, calcium, potassium, hyperpolariza-  
 664 tion, electrical and synaptic currents, respectively. The capacitance of the cell membrane was set to  
 665  $C_m = 1nF$ . Each current is a function of the neuron's membrane potential  $x_m$  and the parameters  
 666 of the circuit such as  $g_{el}$  and  $g_{syn}$ , whose effect on the circuit is considered in the motivational

example of EPI in Fig. 1. Specifically, the currents are the difference in the neuron’s membrane potential and that current type’s reversal potential multiplied by a conductance:

$$h_{leak}(x; z) = g_{leak}(x_m - V_{leak}) \quad (24)$$

$$h_{elec}(x; z) = g_{el}(x_m^{post} - x_m^{pre}) \quad (25)$$

$$h_{syn}(x; z) = g_{syn}S_\infty^{pre}(x_m^{post} - V_{syn}) \quad (26)$$

$$h_{Ca}(x; z) = g_{Ca}M_\infty(x_m - V_{Ca}) \quad (27)$$

$$h_K(x; z) = g_KN(x_m - V_K) \quad (28)$$

$$h_{hyp}(x; z) = g_hH(x_m - V_{hyp}) \quad (29)$$

The reversal potentials were set to  $V_{leak} = -40mV$ ,  $V_{Ca} = 100mV$ ,  $V_K = -80mV$ ,  $V_{hyp} = -20mV$ , and  $V_{syn} = -75mV$ . The other conductance parameters were fixed to  $g_{leak} = 1 \times 10^{-4}\mu S$ .  $g_{Ca}$ ,  $g_K$ , and  $g_{hyp}$  had different values based on fast, intermediate (hub) or slow neuron. Fast:  $g_{Ca} = 1.9 \times 10^{-2}$ ,  $g_K = 3.9 \times 10^{-2}$ , and  $g_{hyp} = 2.5 \times 10^{-2}$ . Intermediate:  $g_{Ca} = 1.7 \times 10^{-2}$ ,  $g_K = 1.9 \times 10^{-2}$ , and  $g_{hyp} = 8.0 \times 10^{-3}$ . Intermediate:  $g_{Ca} = 8.5 \times 10^{-3}$ ,  $g_K = 1.5 \times 10^{-2}$ , and  $g_{hyp} = 1.0 \times 10^{-2}$ .

Furthermore, the Calcium, Potassium, and hyperpolarization channels have time-dependent gating dynamics dependent on steady-state gating variables  $M_\infty$ ,  $N_\infty$  and  $H_\infty$ , respectively.

$$M_\infty = 0.5 \left( 1 + \tanh \left( \frac{x_m - v_1}{v_2} \right) \right) \quad (30)$$

$$\frac{dN}{dt} = \lambda_N(N_\infty - N) \quad (31)$$

$$N_\infty = 0.5 \left( 1 + \tanh \left( \frac{x_m - v_3}{v_4} \right) \right) \quad (32)$$

$$\lambda_N = \phi_N \cosh \left( \frac{x_m - v_3}{2v_4} \right) \quad (33)$$

$$\frac{dH}{dt} = \frac{(H_\infty - H)}{\tau_h} \quad (34)$$

$$H_\infty = \frac{1}{1 + \exp \left( \frac{x_m + v_5}{v_6} \right)} \quad (35)$$

$$\tau_h = 272 - \left( \frac{-1499}{1 + \exp \left( \frac{-x_m + v_7}{v_8} \right)} \right) \quad (36)$$

where we set  $v_1 = 0mV$ ,  $v_2 = 20mV$ ,  $v_3 = 0mV$ ,  $v_4 = 15mV$ ,  $v_5 = 78.3mV$ ,  $v_6 = 10.5mV$ ,  $v_7 = -42.2mV$ ,  $v_8 = 87.3mV$ ,  $v_9 = 5mV$ , and  $v_{th} = -25mV$ . These are the same parameter values used in [22].

690 Finally, there is a synaptic gating variable as well:

$$S_\infty = \frac{1}{1 + \exp\left(\frac{v_{th} - x_m}{v_0}\right)} \quad (37)$$

691 When the dynamic gating variables are considered, this is actually a 15-dimensional nonlinear  
692 dynamical system.

693 In order to measure the frequency of the hub neuron during EPI, the STG model was simulated  
694 for  $T = 500$  time steps of  $dt = 25ms$ . In EPI, since gradients are taken through the simulation  
695 process, the number of time steps are kept as modest if possible. The chosen  $dt$  and  $T$  were the  
696 most computationally convenient choices yielding accurate frequency measurement.

697 Our original approach to measuring frequency was to take the max of the fast Fourier transform  
698 (FFT) of the simulated time series. There are a few key considerations here. One is resolution  
699 in frequency space. Each FFT entry will correspond to a signal frequency of  $\frac{F_s k}{N}$ , where  $N$  is  
700 the number of samples used for the FFT,  $F_s = \frac{1}{dt}$ , and  $k \in [0, 1, \dots, N - 1]$ . Our resolution is  
701 improved by increasing  $N$  and decreasing  $dt$ . Increasing  $N = T - b$ , where  $b$  is some fixed number  
702 of buffer burn-in initialization samples, necessitates an increase in simulation time steps  $T$ , which  
703 directly increases computational cost. Increasing  $F_s$  (decreasing  $dt$ ) increases system approximation  
704 accuracy, but requires more time steps before a full cycle is observed. At the level of  $dt = 0.025$ ,  
705 thousands of temporal samples were required for resolution of .01Hz. These challenges in frequency  
706 resolution with the discrete Fourier transform motivated the use of an alternative basis of complex  
707 exponentials. Instead, we used a basis of complex exponentials with frequencies from 0.0-1.0 Hz at  
708 0.01Hz resolution,  $\Phi = [0.0, 0.01, \dots, 1.0]^\top$

709 Another consideration was that the frequency spectra of the hub neuron has several peaks. This  
710 was due to high-frequency sub-threshold activity. The maximum frequency was often not the firing  
711 frequency. Accordingly, subthreshold activity was set to zero, and the whole signal was low-pass  
712 filtered with a moving average window of length 20. The signal was subsequently mean centered.  
713 After this pre-processing, the maximum frequency in the filter bank accurately reflected the firing  
714 frequency.

715 Finally, to differentiate through the maximum frequency identification step, we used a sum-of-  
716 powers normalization strategy: Let  $\mathcal{X}_i \in \mathcal{C}^{|\Phi|}$  be the complex exponential filter bank dot products  
717 with the signal  $x_i \in \mathcal{R}^N$ , where  $i \in \{\text{f1}, \text{f2}, \text{hub}, \text{s1}, \text{s2}\}$ . The “frequency identification” vector is

$$u_i = \frac{|\mathcal{X}_i|^\alpha}{\sum_{k=1}^N |\mathcal{X}_i(k)|^\alpha} \quad (38)$$

- 718 The frequency is then calculated as  $\Omega_i = u_i^\top \Phi$  with  $\alpha = 100$ .
- 719 Network syncing, like all other emergent properties in this work, are defined by the emergent  
720 property statistics and values. The emergent property statistics are the first- and second-moments  
721 of the firing frequencies. The first moments are set to 0.55Hz, while the second moments are set to  
722 0.025Hz<sup>2</sup>.

$$E \begin{bmatrix} \Omega_{f1} \\ \Omega_{f2} \\ \Omega_{hub} \\ \Omega_{s1} \\ \Omega_{s2} \\ (\Omega_{f1} - 0.55)^2 \\ (\Omega_{f2} - 0.55)^2 \\ (\Omega_{hub} - 0.55)^2 \\ (\Omega_{s1} - 0.55)^2 \\ (\Omega_{s2} - 0.55)^2 \end{bmatrix} = \begin{bmatrix} 0.55 \\ 0.55 \\ 0.55 \\ 0.55 \\ 0.55 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \end{bmatrix} \quad (39)$$

- 723 For EPI in Fig 2C, we used a real NVP architecture with two coupling layers. Each coupling layer  
724 had two hidden layers of 10 units each, and we mapped onto a support of  $z \in \left[ \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 10 \\ 8 \end{bmatrix} \right]$ . We  
725 have shown the EPI optimization that converged with maximum entropy across 2 random seeds  
726 and augmented Lagrangian coefficient initializations of  $c_0=0$ , 2, and 5.

727 **A.2.2 Primary visual cortex**

- 728 The dynamics of each neural populations average rate  $x = \begin{bmatrix} x_E \\ x_P \\ x_S \\ x_V \end{bmatrix}$  are given by:
- $$\tau \frac{dx}{dt} = -x + [Wx + h]_+^n \quad (40)$$

- 729 Some neuron-types largely lack synaptic projections to other neuron-types [57], and it is popular

<sup>730</sup> to only consider a subset of the effective connectivities [23].

$$W = \begin{bmatrix} W_{EE} & W_{EP} & W_{ES} & 0 \\ W_{PE} & W_{PP} & W_{PS} & 0 \\ W_{SE} & 0 & 0 & W_{SV} \\ W_{VE} & W_{VP} & W_{VS} & 0 \end{bmatrix} \quad (41)$$

<sup>731</sup> By consolidating information from many experimental datasets, Billeh et al. [41] produce estimates  
<sup>732</sup> of the synaptic strength (in mV)

$$M = \begin{bmatrix} 0.36 & 0.48 & 0.31 & 0.28 \\ 1.49 & 0.68 & 0.50 & 0.18 \\ 0.86 & 0.42 & 0.15 & 0.32 \\ 1.31 & 0.41 & 0.52 & 0.37 \end{bmatrix} \quad (42)$$

<sup>733</sup> and connection probability

$$C = \begin{bmatrix} 0.16 & 0.411 & 0.424 & 0.087 \\ 0.395 & .451 & 0.857 & 0.02 \\ 0.182 & 0.03 & 0.082 & 0.625 \\ 0.105 & 0.22 & 0.77 & 0.028 \end{bmatrix} \quad (43)$$

<sup>734</sup> Multiplying these connection probabilities and synaptic efficacies gives us an effective connectivity  
<sup>735</sup> matrix:

$$W_{\text{full}} = C \odot M = \begin{bmatrix} 0.16 & 0.411 & 0.424 & 0.087 \\ 0.395 & .451 & 0.857 & 0.02 \\ 0.182 & 0.03 & 0.082 & 0.625 \\ 0.105 & 0.22 & 0.77 & 0.028 \end{bmatrix} \quad (44)$$

<sup>736</sup> From use the entries of this full effective connectivity matrix that are not considered to be ineffectual.  
<sup>737</sup>

<sup>738</sup> We look at how this four-dimensional nonlinear dynamical model of V1 responds to different inputs,  
<sup>739</sup> and compare the predictions of the linear response to the approximate posteriors obtained through  
<sup>740</sup> EPI. The input to the system is the sum of a baseline input  $b = [1 \ 1 \ 1 \ 1]^T$  and a differential  
<sup>741</sup> input  $dh$ :

$$h = b + dh \quad (45)$$

<sup>742</sup> All simulations of this system had  $T = 100$  time points, a time step  $dt = 5\text{ms}$ , and time constant  
<sup>743</sup>  $\tau = 20\text{ms}$ . And the system was initialized to a random draw  $x(0)_i \sim \mathcal{N}(1, 0.01)$ .

<sup>744</sup> We can describe the dynamics of this system more generally by

$$\dot{x}_i = -x_i + f(u_i) \quad (46)$$

<sup>745</sup> where the input to each neuron is

$$u_i = \sum_j W_{ij} x_j + h_i \quad (47)$$

<sup>746</sup> Let  $F_{ij} = \gamma_i \delta(i, j)$ , where  $\gamma_i = f'(u_i)$ . Then, the linear response is

$$\frac{dx_{ss}}{dh} = F(W \frac{dx_{ss}}{dh} + I) \quad (48)$$

<sup>747</sup> which is calculable by

$$\frac{dx_{ss}}{dh} = (F^{-1} - W)^{-1} \quad (49)$$

<sup>748</sup> The emergent property we considered was the first and second moments of the change in rate  $dx$

<sup>749</sup> between the baseline input  $h = b$  and  $h = b + dh$ . We use the following notation to indicate that

<sup>750</sup> the emergent property statistics were set to the following values:

$$\mathcal{B}(\alpha, y) \leftrightarrow E \begin{bmatrix} dx_{\alpha,ss} \\ (dx_{\alpha,ss} - y)^2 \end{bmatrix} = \begin{bmatrix} y \\ 0.01^2 \end{bmatrix} \quad (50)$$

<sup>751</sup> In the final analysis for this model, we sweep the input one neuron at a time away from the mode

<sup>752</sup> of each inferred distributions  $dh^* = z^* = \text{argmax}_z \log q_\theta(z \mid \mathcal{B}(\alpha, 0.1))$ . The differential responses

<sup>753</sup>  $dx_{\alpha,ss}$  are examined at perturbed inputs  $h = b + dh^* + \Delta h_\alpha u_\alpha$  where  $u_\alpha$  is a unit vector in the

<sup>754</sup> dimension of  $\alpha$  and  $\Delta h_\alpha \in [-15, 15]$ .

<sup>755</sup> For each  $\mathcal{B}(\alpha, y)$  with  $\alpha \in \{E, P, S, V\}$  and  $y \in \{0.1, 0.5\}$ , we ran EPI with five different random

<sup>756</sup> initial seeds using an architecture of four coupling layers, each with two hidden layers of 10 units.

<sup>757</sup> We set  $c_0 = 10^5$ . The support of the learned distribution was restricted to  $z_i \in [-5, 5]$ .

### <sup>758</sup> A.2.3 Superior colliculus

<sup>759</sup> There are four total units: two in each hemisphere corresponding to the Pro/Contra and Anti/Ipsi

<sup>760</sup> populations. Each unit has an activity ( $x_i$ ) and internal variable ( $u_i$ ) related by

$$x_i(t) = \left( \frac{1}{2} \tanh \left( \frac{v_i(t) - \epsilon}{\zeta} \right) + \frac{1}{2} \right) \quad (51)$$

<sup>761</sup>  $\epsilon = 0.05$  and  $\zeta = 0.5$  control the position and shape of the nonlinearity, respectively.

<sup>762</sup> We can order the elements of  $x_i$  and  $v_i$  into vectors  $x$  and  $v$  with elements

$$x = \begin{bmatrix} x_{LP} \\ x_{LA} \\ x_{RP} \\ x_{RA} \end{bmatrix} \quad v = \begin{bmatrix} v_{LP} \\ v_{LA} \\ v_{RP} \\ v_{RA} \end{bmatrix} \quad (52)$$

<sup>763</sup> The internal variables follow dynamics:

$$\tau \frac{dv}{dt} = -v + Wx + h + \sigma dB \quad (53)$$

<sup>764</sup> with time constant  $\tau = 0.09s$  and Gaussian noise  $\sigma dB$  controlled by the magnitude of  $\sigma = 1.0$ . The  
<sup>765</sup> weight matrix has 8 parameters  $sW_P$ ,  $sW_A$ ,  $vW_{PA}$ ,  $vW_{AP}$ ,  $hW_P$ ,  $hW_A$ ,  $dW_{PA}$ , and  $dW_{AP}$  (Fig.  
<sup>766</sup> 4B).

$$W = \begin{bmatrix} sW_P & vW_{PA} & hW_P & dW_{PA} \\ vW_{AP} & sW_A & dW_{AP} & hW_A \\ hW_P & dW_{PA} & sW_P & vW_{PA} \\ dW_{AP} & hW_A & vW_{AP} & sW_A \end{bmatrix} \quad (54)$$

<sup>767</sup> The system receives five inputs throughout each trial, which has a total length of 1.8s.

$$h = h_{\text{rule}} + h_{\text{choice-period}} + h_{\text{light}} \quad (55)$$

<sup>768</sup> There are rule-based inputs depending on the condition,

$$h_{P,\text{rule}}(t) = \begin{cases} I_{P,\text{rule}} \begin{bmatrix} 1 & 0 & 0 & 1 \end{bmatrix}^\top, & \text{if } t \leq 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (56)$$

$$h_{A,\text{rule}}(t) = \begin{cases} I_{A,\text{rule}} \begin{bmatrix} 0 & 1 & 1 & 0 \end{bmatrix}^\top, & \text{if } t \leq 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (57)$$

<sup>770</sup> a choice-period input,

$$h_{\text{choice}}(t) = \begin{cases} I_{\text{choice}} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^\top, & \text{if } t > 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (58)$$

<sup>771</sup> and an input to the right or left-side depending on where the light stimulus is delivered.

$$h_{\text{light}}(t) = \begin{cases} I_{\text{light}} \begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}^\top, & \text{if } t > 1.2s \text{ and Left} \\ I_{\text{light}} \begin{bmatrix} 0 & 0 & 1 & 1 \end{bmatrix}^\top, & \text{if } t > 1.2s \text{ and Right} \\ 0, & t \leq 1.2s \end{cases} \quad (59)$$

772 The input parameterization was fixed to  $I_{P,\text{rule}} = 10$ ,  $I_{A,\text{rule}} = 10$ ,  $I_{\text{choice}} = 2$ , and  $I_{\text{light}} = 1$   
 773 To produce a Bernoulli rate of  $p_{LP}$  in the Left, Pro condition (we can generalize this to either cue,  
 774 or stimulus condition), let  $\hat{p}_i$  be the empirical average steady state (ss) response (final  $x_{LP}$  at end  
 775 of task) over  $M=500$  Gaussian noise draws for a given SC model parameterization  $z_i$ :

$$\hat{p}_i = E_{\sigma dB} [x_{LP,ss} | s = L, c = P, z_i] = \frac{1}{M} \sum_{j=1}^M x_{LP,ss}(s = L, c = P, z_i, \sigma dB_j) \quad (60)$$

776 For the first constraint, the average over posterior samples (from  $q_\theta(z)$ ) to be  $p_{LP}$ :

$$E_{z_i \sim q_\phi} [E_{\sigma dB} [x_{LP,ss} | s = L, c = P, z_i]] = E_{z_i \sim q_\phi} [\hat{p}_i] = p_{LP} \quad (61)$$

777 We can then ask that the variance of the steady state responses across Gaussian draws, is the  
 778 Bernoulli variance for the empirical rate  $\hat{p}_i$ .

$$E_{z \sim q_\phi} [\sigma_{err}^2] = 0 \quad (62)$$

779

$$\sigma_{err}^2 = Var_{\sigma dB} [x_{LP,ss} | s = L, c = P, z_i] - \hat{p}_i(1 - \hat{p}_i) \quad (63)$$

780 We have an additional constraint that the Pro neuron on the opposite hemisphere should have the  
 781 opposite value. We can enforce this with a final constraint:

$$E_{z \sim q_\phi} [d_P] = 1 \quad (64)$$

782

$$E_{\sigma dB} [(x_{LP,ss} - x_{RP,ss})^2 | s = L, c = P, z_i] \quad (65)$$

783 We refer to networks obeying these constraints as Bernoulli, winner-take-all networks. Since the  
 784 maximum variance of a random variable bounded from 0 to 1 is the Bernoulli variance ( $\hat{p}(1 - \hat{p})$ ),  
 785 and the maximum squared difference between two variables bounded from 0 to 1 is 1, we do not  
 786 need to control the second moment of these test statistics. In reality, these variables are dynamical  
 787 system states and can only exponentially decay (or saturate) to 0 (or 1), so the Bernoulli variance  
 788 error and squared difference constraints can only be undershot. This is important to be mindful  
 789 of when evaluating the convergence criteria. Instead of using our usual hypothesis testing criteria  
 790 for convergence to the emergent property, we set a slack variable threshold for these technically  
 791 infeasible constraints to 0.05.

792 Training DSNs to learn distributions of dynamical system parameterizations that produce Bernoulli  
 793 responses at a given rate (with small variance around that rate) was harder to do than expected.

794 There is a pathology in this optimization setup, where the learned distribution of weights is bimodal  
 795 attributing a fraction  $p$  of the samples to an expansive mode (which always sends  $x_{LP}$  to 1), and a  
 796 fraction  $1 - p$  to a decaying mode (which always sends  $x_{LP}$  to 0). This pathology was avoided using  
 797 an inequality constraint prohibiting parameter samples that resulted in low variance of responses  
 798 across noise.

799 In total, the emergent property of rapid task switching accuracy at level  $p$  was defined as

$$\mathcal{B}(p) \leftrightarrow \begin{bmatrix} \hat{p}_P \\ \hat{p}_A \\ (\hat{p}_P - p)^2 \\ (\hat{p}_A - p)^2 \\ \sigma_{P,err}^2 \\ \sigma_{A,err}^2 \\ d_P \\ d_A \end{bmatrix} = \begin{bmatrix} p \\ p \\ 0.15^2 \\ 0.15^2 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \quad (66)$$

800 For each accuracy level  $p$ , we ran EPI for 10 different random seeds and selected the maximum  
 801 entropy solution using an architecture of 10 planar flows with  $c_0 = 2$ . The support of  $z$  was  $\mathcal{R}^8$ .

#### 802 A.2.4 Rank-1 RNN

803 Recent work establishes a link between RNN connectivity weights and the resulting dynamical  
 804 responses of the network, using dynamic mean field theory (DMFT) [25]. Specifically, DMFT  
 805 describes the properties of activity in infinite-size neural networks given a distribution on the  
 806 connectivity weights. In such a model, the connectivity of a rank-1 RNN (which was sufficient for  
 807 our task), has weight matrix  $W$ , which is the sum of a random component with strength determined  
 808 by  $g$  and a structured component determined by the outer product of vectors  $m$  and  $n$ :

$$W = g\chi + \frac{1}{N}mn^\top, \quad (67)$$

809 where the activity  $x$  evolves as and  $I(t)$  is some input,  $\phi$  is the tanh nonlinearity, and  $\chi_{ij} \sim \mathcal{N}(0, \frac{1}{N})$ .  
 810 The entries of  $m$  and  $n$  are drawn from Gaussian distributions  $m_i \sim \mathcal{N}(M_m, 1)$  and  $n_i \sim \mathcal{N}(M_n, 1)$ .  
 811 From such a parameterization, this theory produces consistency equations for the dynamic mean  
 812 field variables in terms of parameters like  $g$ ,  $M_m$ , and  $M_n$ , which we study in Section 3.5. That  
 813 is the dynamic mean field variables (e.g. the activity along a vector  $\kappa_v$ , the total variance

814  $\Delta_0$ , structured variance  $\Delta_\infty$ , and the chaotic variance  $\Delta_T$ ) are written as functions of one another  
815 in terms of connectivity parameters. The values of these variables can be used obtained using a  
816 nonlinear system of equations solver. These dynamic mean field variables are then cast as task-  
817 relevant variables with respect to the context of the provided inputs. Mastrogiuseppe et al. designed  
818 low-rank RNN connectivities via minimalist connectivity parameters to solve canonical tasks from  
819 behavioral neuroscience.

820 We consider the DMFT equation solver as a black box that takes in a low-rank parameterization  $z$   
821 (e.g.  $z = [g \quad M_m \quad M_n]$ ) and outputs the values of the dynamic mean field variables, of which we  
822 cast  $\kappa_w$  and  $\Delta_T$  as task-relevant variables  $\mu_{\text{post}}$  and  $\sigma_{\text{post}}^2$  in the Gaussian posterior conditioning  
823 toy example. Importantly, the solution produced by the solver is differentiable with respect to the  
824 input parameters, allowing us to use DMFT to calculate the emergent property statistics in EPI  
825 to learn distributions on such connectivity parameters of RNNs that execute tasks.

826 Specifically, we solve for the mean field variables  $\kappa_w$ ,  $\kappa_n$ ,  $\Delta_0$  and  $\Delta_\infty$ , where the readout is nominally  
827 chosen to point in the unit orthant  $w = [1 \quad \dots \quad 1]^\top$ . The consistency equations for these variables  
828 in the presence of an constant input  $I(t) = y - (n - M_n)$  can be derived following [25] are

$$\begin{aligned} \kappa_w &= F(\kappa_w, \kappa_n, \Delta_0, \Delta_\infty) = M_m \kappa_n + y \\ \kappa_n &= G(\kappa_w, \kappa_n, \Delta_0, \Delta_\infty) = M_n \langle [\phi_i] \rangle + \langle [\phi'_i] \rangle \\ \frac{\Delta_0^2 - \Delta_\infty^2}{2} &= H(\kappa_w, \kappa_n, \Delta_0, \Delta_\infty) = g^2 \left( \int \mathcal{D}z \Phi^2(\kappa_w + \sqrt{\Delta_0} z) - \int \mathcal{D}z \int \mathcal{D}x \Phi(\kappa_w + \sqrt{\Delta_0 - \Delta_\infty} x + \sqrt{\Delta_\infty} z) \right) \\ &\quad + (\kappa_n^2 + 1)(\Delta_0 - \Delta_\infty) \\ \Delta_\infty &= L(\kappa_w, \kappa_n, \Delta_0, \Delta_\infty) = g^2 \int \mathcal{D}z \left[ \int \mathcal{D}x \phi(\kappa_w + \sqrt{\Delta_0 - \Delta_\infty} x + \sqrt{\Delta_\infty} z) \right]^2 + \kappa_n^2 + 1 \end{aligned} \tag{68}$$

829 where  $z$  here is a gaussian integration variable. We can solve these equations by simulating the  
830 following Langevin dynamical system.

$$\begin{aligned} x(t) &= \frac{\Delta_0(t)^2 - \Delta_\infty(t)^2}{2} \\ \Delta_0(t) &= \sqrt{2x(t) + \Delta_\infty(t)^2} \\ \dot{\kappa}_w(t) &= -\kappa_w(t) + F(\kappa_w(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \\ \dot{\kappa}_n(t) &= -\kappa_n + G(\kappa_w(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \\ \dot{x}(t) &= -x(t) + H(\kappa_w(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \\ \dot{\Delta_\infty}(t) &= -\Delta_\infty(t) + L(\kappa_w(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \end{aligned} \tag{69}$$

831 Then, the temporal variance, which is necessary for the Gaussian posterior conditioning example,  
832 is simply calculated via

$$\Delta_T = \Delta_0 - \Delta_\infty \quad (70)$$

833 **A.3 Supplementary Figures**

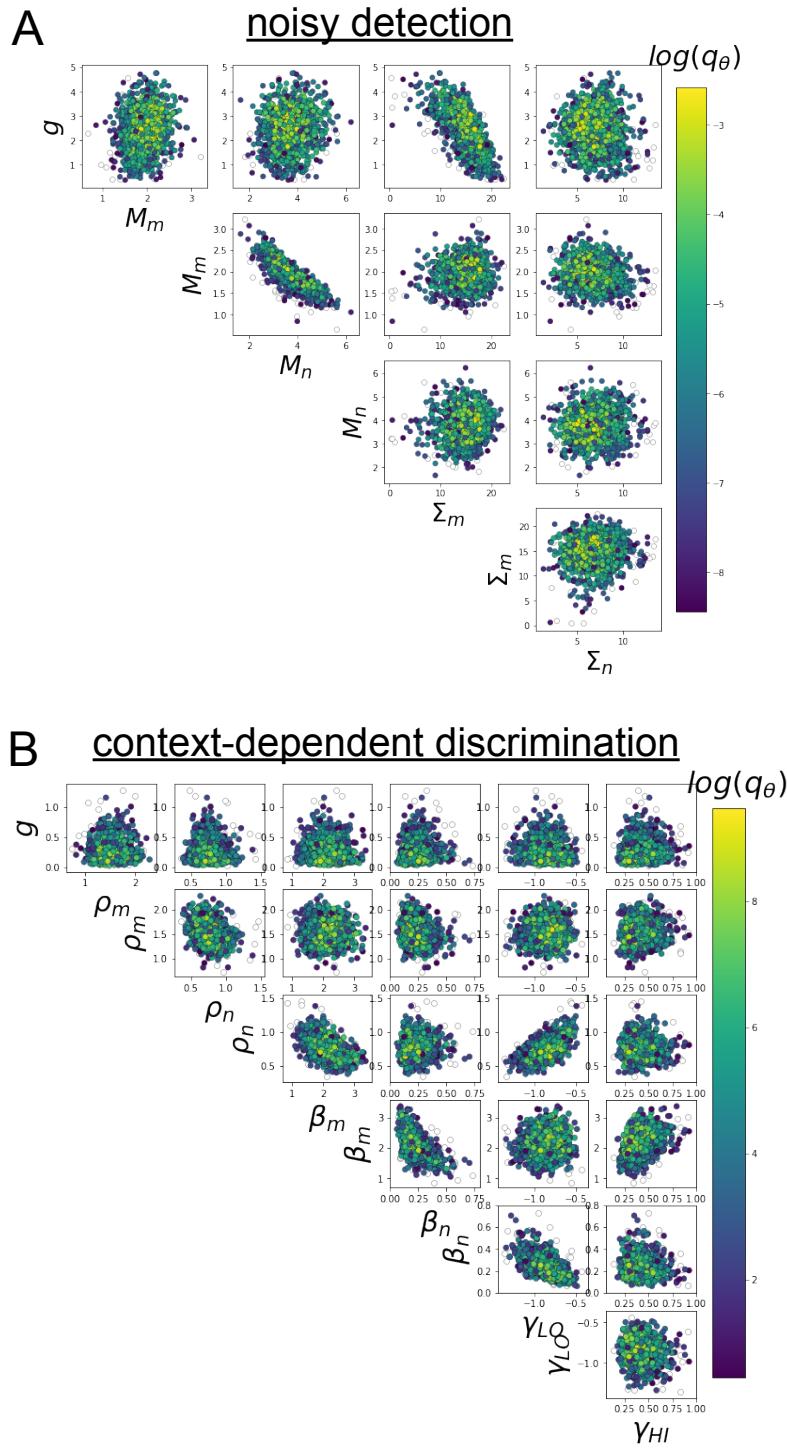


Fig. S1: A. EPI for rank-1 networks doing discrimination. B. EPI for rank-2 networks doing context-dependent discrimination.