

Interrogating theoretical models of neural computation with deep inference  
Sean R. Bittner<sup>1</sup>, Agostina Palmigiano<sup>1</sup>, Alex T. Piet<sup>2,3</sup>, Chunyu A. Duan<sup>4</sup>, Carlos D. Brody<sup>2,3,5</sup>,  
Kenneth D. Miller<sup>1</sup>, and John P. Cunningham<sup>6</sup>.

<sup>1</sup>Department of Neuroscience, Columbia University,

<sup>2</sup>Princeton Neuroscience Institute,

<sup>3</sup>Princeton University,

<sup>4</sup>Institute of Neuroscience, Chinese Academy of Sciences,

<sup>5</sup>Howard Hughes Medical Institute,

<sup>6</sup>Department of Statistics, Columbia University

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

<sup>2</sup> A 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  
<sup>5</sup> offer insights into neural computation. The operation of these circuits, like all models, critically  
<sup>6</sup> depends on the choices of model parameters. Historically, the gold standard has been to analyt-  
<sup>7</sup> ically derive the relationship between model parameters and computational properties. However,  
<sup>8</sup> this enterprise quickly becomes infeasible as biologically realistic constraints are included into the  
<sup>9</sup> model increasing its complexity, often resulting in *ad hoc* approaches to understanding the relation-  
<sup>10</sup> ship between model and computation. We bring recent machine learning techniques – the use of  
<sup>11</sup> deep generative models for probabilistic inference – to bear on this problem, learning distributions  
<sup>12</sup> of parameters that produce the specified properties of computation. Importantly, the techniques  
<sup>13</sup> we introduce offer a principled means to understand the implications of model parameter choices  
<sup>14</sup> on computational properties of interest. We motivate this methodology with a worked example  
<sup>15</sup> analyzing sensitivity in the stomatogastric ganglion. We then use it to go beyond linear theory  
<sup>16</sup> of neuron-type input-responsivity in a model of primary visual cortex, gain a mechanistic under-  
<sup>17</sup> standing of rapid task switching in superior colliculus models, and attribute error to connectivity  
<sup>18</sup> properties in recurrent neural networks solving a simple mathematical task. More generally, this  
<sup>19</sup> work suggests a departure from realism vs tractability considerations, towards the use of modern  
<sup>20</sup> machine learning for sophisticated interrogation of biologically relevant models.

## 21 2 Introduction

22 The fundamental practice of theoretical neuroscience is to use a mathematical model to understand  
23 neural computation, whether that computation enables perception, action, or some intermediate  
24 processing [1]. A neural computation is systematized with a set of equations – the model – and  
25 these equations are motivated by biophysics, neurophysiology, and other conceptual considerations.  
26 The function of this system is governed by the choice of model parameters, which when configured  
27 in a particular way, give rise to a measurable signature of a computation. The work of analyzing a  
28 model then requires solving the inverse problem: given a computation of interest, how can we reason  
29 about these particular parameter configurations? The inverse problem is crucial for reasoning about  
30 likely parameter values, uniquenesses and degeneracies, attractor states and phase transitions, and  
31 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 (which often adopt  
34 approaches from statistical physics) include our field’s understanding of memory capacity in asso-  
35 ciative neural networks [2], chaos and autocorrelation timescales in random neural networks [3],  
36 the paradoxical effect [4], and decision making [5]. Unfortunately, as circuit models include more  
37 biological realism, theory via analytical derivation becomes intractable. This creates an unfavor-  
38 able tradeoff. On the one hand, one may tractably analyze systems of equations with unrealistic  
39 assumptions (for example symmetry or gaussianity), mathematically formalizing how parameters  
40 affect computation in a too-simple model. On the other hand, one may choose a more biologically  
41 accurate, scientifically relevant model at the cost of *ad hoc* approaches to analysis (such as sim-  
42 ply examining simulated activity), potentially resulting in bad inference of parameters and thus  
43 erroneous scientific predictions or conclusions.

44 Of course, this same tradeoff has been confronted in many scientific fields characterized by the  
45 need to do inference in complex models. In response, the machine learning community has made  
46 remarkable progress in recent years, via the use of deep neural networks as a powerful inference  
47 engine: a flexible function family that can map observed phenomena (in this case the measurable  
48 signal of some computation) back to probability distributions quantifying the likely parameter  
49 configurations. One celebrated example of this approach from machine learning, of which we  
50 draw key inspiration for this work, is the variational autoencoder [6, 7], which uses a deep neural  
51 network to induce an (approximate) posterior distribution on hidden variables in a latent variable

model, given data. Indeed, these tools have been used to great success in neuroscience as well, in particular for interrogating parameters (sometimes treated as hidden states) in models of both cortical population activity [8, 9, 10, 11] and animal behavior [12, 13, 14]. These works have used deep neural networks to expand the expressivity and accuracy of statistical models of neural data [15].

However, these inference tools have not significantly influenced the study of theoretical neuroscience 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 theoreticians work carefully to construct a model that has biological relevance, such a model as a result often does 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 [16]. 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 [17, 18, 19]. 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 [20]. 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

[21]. 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 [22], 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 infinite neurons). First, we use EPI to produce a set of verifiable hypotheses of input-responsivity in a four neuron-type dynamical model of primary visual cortex; we then validate these hypotheses in the model. Second, we demonstrated how the systematic application of EPI to levels of task performance can generate experimentally testable hypotheses regarding connectivity in superior colliculus. Third, we use EPI to uncover the sources of error in a low-rank recurrent neural network executing a simple mathematical task. The novel scientific insights offered by EPI contextualize and clarify the previous studies exploring these models [23, 24, 25, 26], and more generally, these results point to the value of deep inference for the interrogation of biologically relevant models.

We note that, during our preparation and early presentation of this work [27, 28], another work has arisen with broadly similar goals: bringing statistical inference to mechanistic models of neural circuits [29, 30]. We are encouraged by this general problem being recognized by others in the community, and we emphasize that these works offer complementary neuroscientific contributions (different theoretical models of focus) and use different technical methodologies (ours is built on our prior work [20], theirs similarly [31]). These distinct methodologies and scientific investigations emphasize the increased importance and timeliness of both works.

## 3 Results

### 3.1 Motivating emergent property inference of theoretical models

Consideration of the typical workflow of theoretical modeling clarifies the need for emergent property inference. First, one designs or chooses an existing model that, it is hypothesized, captures the computation of interest. To ground this process in a well-known example, consider the stomatogastric ganglion (STG) of crustaceans, a small neural circuit which generates multiple rhythmic muscle activation patterns for digestion [32]. Despite full knowledge of STG connectivity and a

114 precise characterization of its rhythmic pattern generation, biophysical models of the STG have  
 115 complicated relationships between circuit parameters and neural activity [22, 33]. A model of the  
 116 STG [23] is shown schematically in Figure 1A, and note that the behavior of this model will be crit-  
 117 ically dependent on its parameterization – the choices of conductance parameters  $z = [g_{el}, g_{synA}]$ .  
 118 Specifically, the two fast neurons ( $f_1$  and  $f_2$ ) mutually inhibit one another, and oscillate at a faster  
 119 frequency than the mutually inhibiting slow neurons ( $s_1$  and  $s_2$ ). The hub neuron (hub) couples  
 120 with either the fast or slow population or both.  
 121 Second, once the model is selected, one defines the emergent property, the measurable signal of  
 122 scientific interest. To continue our running STG example, one such emergent property is the  
 123 phenomenon of *network syncing* – in certain parameter regimes, the frequency of the hub neuron  
 124 matches that of the fast and slow populations at an intermediate frequency. This emergent property  
 125 is shown in Figure 1A at a frequency of 0.53Hz.  
 126 Third, qualitative parameter analysis ensues: since precise mathematical analysis is intractable in  
 127 this model, a brute force sweep of parameters is done [23]. Subsequently, a qualitative description  
 128 is formulated to describe the different parameter configurations that lead to the emergent property.  
 129 In this last step lies the opportunity for a precise quantification of the emergent property as a  
 130 statistical feature of the model. Once we have such a methodology, we can infer a probability  
 131 distribution over parameter configurations that produce this emergent property.  
 132 Before presenting technical details (in the following section), let us understand emergent property  
 133 inference schematically: EPI (Fig. 1A gray box) takes, as input, the model and the specified  
 134 emergent property, and as its output, produces the parameter distribution shown in Figure 1B.  
 135 This distribution – represented for clarity as samples from the distribution – is then a scientifically  
 136 meaningful and mathematically tractable object. In the STG model, this distribution can be  
 137 specifically queried to reveal the prototypical parameter configuration for network syncing (the  
 138 mode; Figure 1B yellow star), and how network syncing decays based on changes away from the  
 139 mode. The eigenvectors (of the Hessian of the distribution at the mode) quantitatively formalize  
 140 the robustness of network syncing (Fig. 1B solid ( $v_1$ ) and dashed ( $v_2$ ) black arrows). Indeed,  
 141 samples equidistant from the mode along these EPI-identified dimensions of sensitivity ( $v_1$ ) and  
 142 degeneracy ( $v_2$ ) agree with error contours (Fig. 1B, contours) and have diminished or preserved  
 143 network syncing, respectively (Figure 1B inset and activity traces) (see Section 5.2.1).

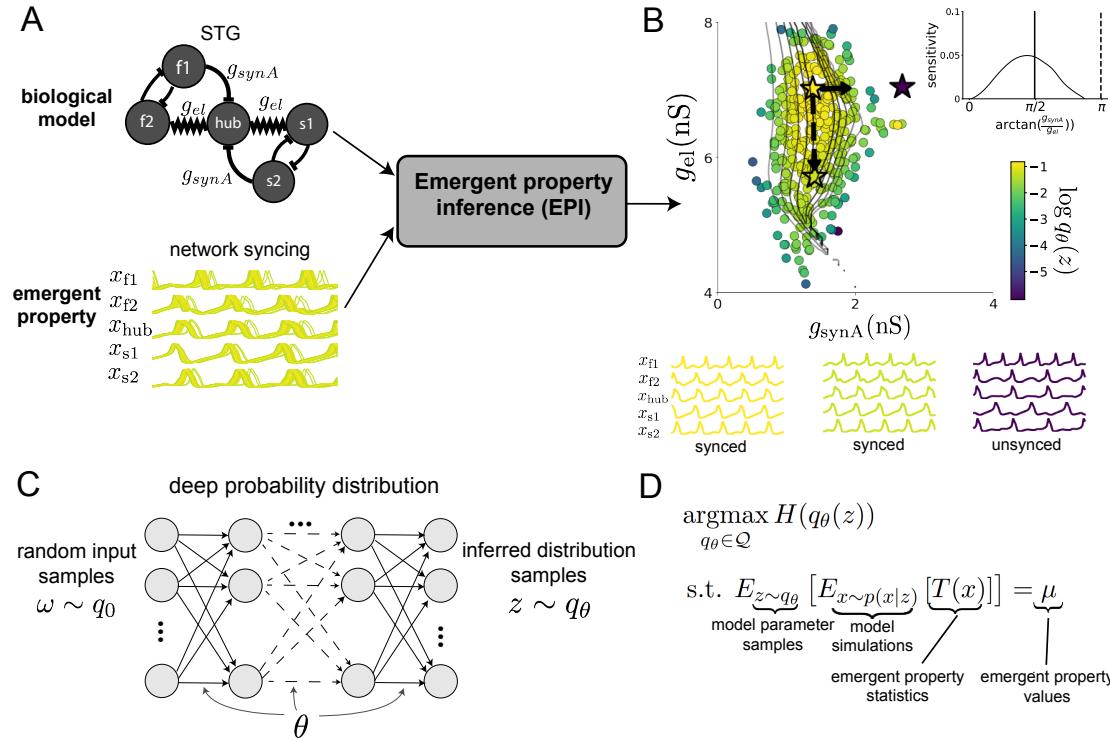


Figure 1: Emergent property inference (EPI) in the stomatogastric ganglion. A. For a choice of model (STG) and emergent property (network syncing), emergent property inference (EPI, gray box) learns a distribution of the model parameters  $z = [g_{el}, g_{synA}]$  producing network syncing. In the STG model, jagged connections indicate electrical coupling having electrical conductance  $g_{el}$ . Other connections in the diagram are inhibitory synaptic projections having strength  $g_{synA}$  onto the hub neuron, and  $g_{synB} = 5\text{nS}$  for mutual inhibitory connections. Network syncing traces are colored by log probability density of their generating parameters (stars) in the EPI-inferred distribution. B. The EPI distribution of STG model parameters producing network syncing. Samples are colored by log probability density. Distribution contours of emergent property value error are shown at levels of  $2.5 \times 10^{-5}$ ,  $5 \times 10^{-5}$ ,  $1 \times 10^{-4}$ ,  $2 \times 10^{-4}$ , and  $4 \times 10^{-4}$  (dark to light gray). Eigenvectors of the Hessian at the mode of the inferred distribution are indicated as  $v_1$  (solid) and  $v_2$  (dashed) with lengths scaled by the square root of the absolute value of their eigenvalues. 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.  $v_1$  is sensitive to network syncing ( $p < 10^{-4}$ ), while  $v_2$  is not ( $p = 0.67$ ) (see Section 5.2.1). C. Deep probability distributions map a latent random variable  $w$  through a deep neural network with weights and biases  $\theta$  to parameters  $z = f_\theta(w)$  distributed as  $q_\theta(z)$ . D. EPI optimization: To learn the EPI distribution  $q_\theta(z)$  of model parameters that produce an emergent property, the emergent property statistics  $T(x)$  are set in expectation over model parameter samples  $z \sim q_\theta(z)$  and model simulations  $x \sim p(x | z)$  to emergent property values  $\mu$ .

<sup>144</sup> **3.2 A deep generative modeling approach to emergent property inference**

<sup>145</sup> Emergent property inference (EPI) systematizes the three-step procedure of the previous section.  
<sup>146</sup> First, we consider the model as a coupled set of differential (and potentially stochastic) equations  
<sup>147</sup> [23]. In the running STG example, the model activity  $x = [x_{f1}, x_{f2}, x_{hub}, x_{s1}, x_{s2}]$  is the membrane  
<sup>148</sup> potential for each neuron, which evolves according to the biophysical conductance-based equation:

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

<sup>149</sup> where  $C_m = 1\text{nF}$ , and  $h_{leak}$ ,  $h_{Ca}$ ,  $h_K$ ,  $h_{hyp}$ ,  $h_{elec}$ , and  $h_{syn}$  are the leak, calcium, potassium, hyper-  
<sup>150</sup> polarization, electrical, and synaptic currents, all of which have their own complicated dependence  
<sup>151</sup> on  $x$  and  $z = [g_{el}, g_{synA}]$  (see Section 5.2.1).

<sup>152</sup> Second, we define the emergent property, which as above is network syncing: oscillation of the  
<sup>153</sup> entire population at an intermediate frequency of our choosing (Figure 1A bottom). Quantifying  
<sup>154</sup> this phenomenon is straightforward: we define network syncing to be that each neuron’s spiking  
<sup>155</sup> frequency – denoted  $\omega_{f1}(x)$ ,  $\omega_{f2}(x)$ , etc. – is close to an intermediate frequency of 0.53Hz. Math-  
<sup>156</sup> ematically, we achieve this via constraints on the mean and variance of  $\omega_\alpha(x)$  for each neuron  
<sup>157</sup>  $\alpha \in \{f1, f2, hub, s1, s2\}$ :

$$\mathbb{E}[T(x)] \triangleq \mathbb{E} \begin{bmatrix} \omega_{f1}(x) \\ \vdots \\ (\omega_{f1}(x) - 0.53)^2 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0.53 \\ \vdots \\ 0.025^2 \\ \vdots \end{bmatrix} \triangleq \mu, \quad (2)$$

<sup>158</sup> which completes the quantification of the emergent property.

<sup>159</sup> Third, we perform emergent property inference: we find a distribution over parameter configura-  
<sup>160</sup> tions  $z$ , and insist that samples from this distribution produce the emergent property; in other  
<sup>161</sup> words, they obey the constraints introduced in Equation 2. This distribution will be chosen from  
<sup>162</sup> a family of probability distributions  $\mathcal{Q} = \{q_\theta(z) : \theta \in \Theta\}$ , defined by a deep generative distribution  
<sup>163</sup> of the normalizing flow class [17, 18, 19] – neural networks which transform a simple distribution  
<sup>164</sup> into a suitably complicated distribution (as is needed here). This deep distribution is represented  
<sup>165</sup> in Figure 1C (see Section 5.1). Then, mathematically, we must solve the following optimization  
<sup>166</sup> program:

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

where  $T(x), \mu$  are defined as in Equation 2, 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 [34, 35, 20, 36], but we emphasize that the EPI methodology is unaffected by this choice (although the results of course 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 (Fig. S4). 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 5.1.2). Further validation of EPI is available in the supplementary materials, where we analyze a simpler model for which ground-truth statements can be made (Section 5.1.1). In relation to broader methodology, inspection of the EPI objective reveals a natural relationship to posterior inference. Specifically, EPI executes variational inference in an exponential family model, the sufficient statistics and mean parameter of which are defined by the emergent property statistics and values, respectively (see Section 5.1.4). Equipped with this method, we now prove out the value of EPI by using it to investigate and produce novel insights about three prominent models in neuroscience.

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

Dynamical models of excitatory (E) and inhibitory (I) populations with supralinear input-output function have succeeded in explaining a host of experimentally documented phenomena. In a regime characterized by inhibitory stabilization of strong recurrent excitation, these models give rise to paradoxical responses [4], selective amplification [37], surround suppression [38] and normalization [39]. Despite their strong predictive power, E-I circuit models rely on the assumption that inhibition can be studied as an indivisible unit. However, experimental evidence shows that inhibition is composed of distinct elements – parvalbumin (P), somatostatin (S), VIP (V) – composing 80% of GABAergic interneurons in V1 [40, 41, 42], and that these inhibitory cell types follow specific connectivity patterns (Fig. 2A) [43]. Recent theoretical advances [24, 44, 45], have only started

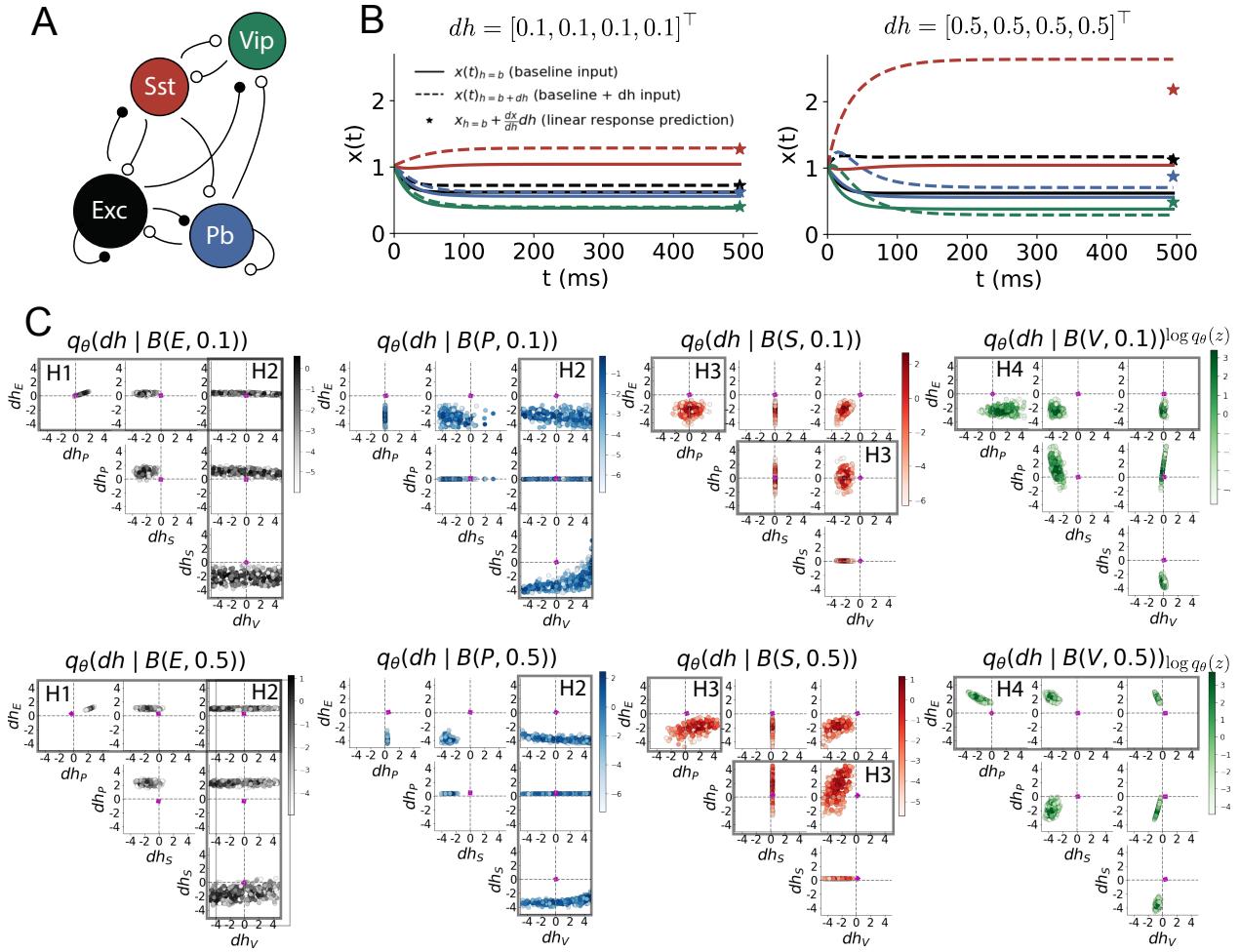


Figure 2: Hypothesis generation through EPI in a V1 model. A. Four-population model of primary visual cortex with excitatory (black), parvalbumin (blue), somatostatin (red), and VIP (green) neurons. Some neuron-types largely do not form synaptic projections to others (excitatory and inhibitory projections filled and unfilled, respectively). B. Linear response predictions become inaccurate with greater input strength. V1 model simulations for input (solid)  $h = b$  and (dashed)  $h = b + dh$ . 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).

198 to address the consequences of this multiplicity in the dynamics of V1, strongly relying on linear  
 199 theoretical tools. Here, we go beyond linear theory by systematically generating and evaluating hy-  
 200 potheses of circuit model function using EPI distributions of neuron-type inputs producing various  
 201 neuron-type population responses.

202 Specifically, we consider a four-dimensional circuit model with dynamical state given by the firing  
 203 rate  $x$  of each neuron-type population  $x = [x_E, x_P, x_S, x_V]^\top$ . Given a time constant of  $\tau = 20$  ms  
 204 and a power  $n = 2$ , the dynamics are driven by the rectified and exponentiated sum of recurrent  
 205 ( $Wx$ ) and external  $h$  inputs:

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

206 The effective connectivity weights  $W$  were obtained from experimental recordings of publicly avail-  
 207 able datasets of mouse V1 [46, 47] (see Section 5.2.2). The input  $h = b + dh$  is comprised of a  
 208 baseline input  $b = [b_E, b_P, b_S, b_V]^\top$  and a differential input  $dh = [dh_E, dh_P, dh_S, dh_V]^\top$  to each  
 209 neuron-type population. Throughout subsequent analyses, the baseline input is  $b = [1, 1, 1, 1]^\top$ .

210 With this model, we are interested in the differential responses of each neuron-type population to  
 211 changes in input  $dh$ . Initially, we studied the linearized response of the system to input  $\frac{dx_{ss}}{dh}$  at the  
 212 steady state response  $x_{ss}$ , i.e. a fixed point. All analyses of this model consider the steady state  
 213 response, so we drop the notation  $ss$  from here on. While this linearization accurately predicts  
 214 differential responses  $dx = [dx_E, dx_P, dx_S, dx_V]^\top$  for small differential inputs to each population  
 215  $dh = [0.1, 0.1, 0.1, 0.1]^\top$  (Fig 2B left), the linearization is a poor predictor in this nonlinear model  
 216 more generally (Fig. 2B right). Currently available approaches to deriving the steady state response  
 217 of the system are limited.

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

$$\mathcal{B}(\alpha, y) \triangleq \mathbb{E} \begin{bmatrix} dx_\alpha \\ (dx_\alpha - y)^2 \end{bmatrix} = \begin{bmatrix} y \\ 0.01^2 \end{bmatrix}. \quad (5)$$

224 We maintain the notation  $\mathcal{B}(\cdot)$  throughout the rest of the study as short hand for emergent property,

which represents a different signature of computation in each application.

Using EPI, we inferred the distribution of  $dh$  shown in Figure 2C producing  $\mathcal{B}(\alpha, y)$ . Columns correspond to inferred distributions of excitatory ( $\alpha = E$ , red), parvalbumin ( $\alpha = P$ , blue), somatostatin ( $\alpha = S$ , red) and VIP ( $\alpha = V$ , green) neuron-type response increases, while each row corresponds to increase amounts of  $y \in \{0.1, 0.5\}$ . For each pair of parameters, we show the two-dimensional marginal distribution of samples colored by  $\log q_\theta(dh | \mathcal{B}(\alpha, y))$ . The inferred distributions immediately suggest four hypotheses:

232

- 233 H1: as is intuitive, each neuron-type's firing rate should be sensitive to that neuron-type's  
234 direct input (e.g. Fig. 2C H1 gray boxes indicate low variance in  $dh_E$  when  $\alpha = E$ . Same  
235 observation in all inferred distributions);
  - 236 H2: the E- and P-populations should be largely unaffected by input to the V-population (Fig.  
237 2C H2 gray boxes indicate high variance in  $dh_V$  when  $\alpha \in \{E, P\}$ );
  - 238 H3: the S-population should be largely unaffected by input to the P-population (Fig. 2C H3  
239 gray boxes indicate high variance in  $dh_P$  when  $\alpha = S$ );
  - 240 H4: there should be a nonmonotonic response of the V-population with input to the E-  
241 population (Fig. 2C H4 gray boxes indicate that negative  $dh_E$  should result in small  $dx_V$ ,  
242 but positive  $dh_E$  should elicit a larger  $dx_V$ );
- 243 We evaluate these hypotheses by taking perturbations in individual neuron-type input  $\delta h_\alpha$  away  
244 from the modes of the inferred distributions at  $y = 0.1$

$$dh^* = z^* = \underset{z}{\operatorname{argmax}} \log q_\theta(z | \mathcal{B}(\alpha, 0.1)). \quad (6)$$

245 Here  $\delta x_\alpha$  is the change in steady state response of the system with input  $h = b + dh^* + \delta h_\alpha \hat{u}_\alpha$   
246 compared to  $h = b + dh^*$ , where  $\hat{u}_\alpha$  is a unit vector in the dimension of  $\alpha$ . The EPI-generated  
247 hypotheses are confirmed (for details, see Section 5.2.2):

- 248 H1: the neuron-type responses are sensitive to their direct inputs (Fig. 3A black, 3B blue,  
249 3C red, 3D green);
- 250 H2: the E- and P-populations are not affected by  $\delta h_V$  (Fig. 3A green, 3B green);
- 251 H3: the S-population is not affected by  $\delta h_P$  (Fig. 3C blue);
- 252 H4: the V-population exhibits a nonmonotonic response to  $\delta h_E$  (Fig. 3D black), and is in  
253 fact the only population to do so (Fig. 3A-C black).

254 These hypotheses were in stark contrast to what was available to us via traditional analytical

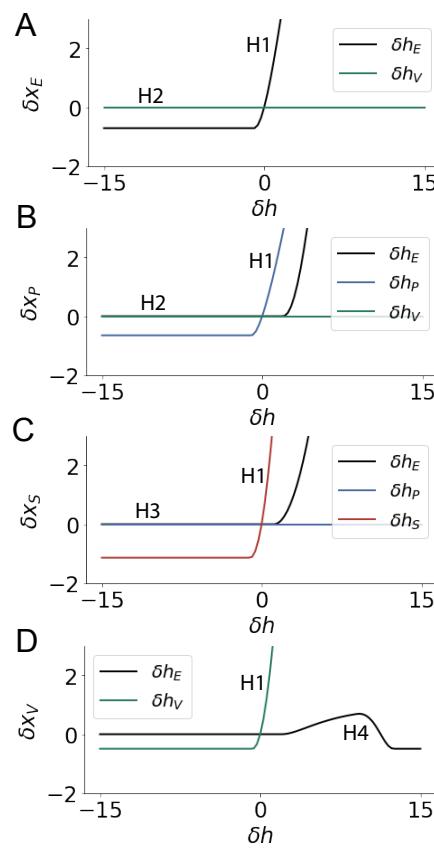


Figure 3: Confirming EPI generated hypotheses in V1. A. Differential responses  $\delta x_E$  by the E-population to changes in individual input  $\delta h_\alpha \hat{u}_\alpha$  away from the mode of the EPI distribution  $dh^*$ . B-D Same plots for the P-, S-, and V-populations. Labels H1, H2, H3,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

linear prediction (Fig. 2C, magenta, see Section 5.2.2). To this point, we have shown the utility of EPI on relatively low-level emergent properties like network syncing and differential neuron-type population responses. In the remainder of the study, we focus on using EPI to understand models of more abstract cognitive function.

### 3.4 Identifying neural mechanisms of flexible task switching

In a rapid task switching experiment [48], rats were explicitly cued on each trial to either orient towards a visual stimulus in the Pro (P) task or orient away from a visual stimulus in the Anti (A) task (Fig. 4a). Neural recordings in the midbrain superior colliculus (SC) exhibited two populations of neurons that simultaneously represented both task context (Pro or Anti) and motor response (contralateral or ipsilateral to the recorded side): the Pro/Contra and Anti/Ipsi neurons [25]. Duan et al. proposed a model of SC that, like the V1 model analyzed in the previous section, is a four-population dynamical system. We analyzed this model, where the neuron-type populations are functionally-defined as the Pro- and Anti-populations in each hemisphere (left (L) and right (R)), their connectivity is parameterized geometrically (Fig. 4B). The input-output function of this model is chosen such that the population responses  $x = [x_{LP}, x_{LA}, x_{RP}, x_{RA}]^\top$  are bounded

270 from 0 to 1 giving rise to high (1) or low (0) responses at the end of the trial:

$$x_\alpha = \left( \frac{1}{2} \tanh \left( \frac{u_\alpha - \epsilon}{\zeta} \right) + \frac{1}{2} \right) \quad (7)$$

271 where  $\epsilon = 0.05$  and  $\zeta = 0.5$ . The dynamics evolve with timescale  $\tau = 0.09$  via an internal variable  
272  $u$  governed by connectivity weights  $W$

$$\tau \frac{du}{dt} = -u + Wx + h + \sigma dB \quad (8)$$

273 with gaussian noise of variance  $\sigma^2 = 1$ . The input  $h$  is comprised of a cue-dependent input to the  
274 Pro or Anti populations, a stimulus orientation input to either the Left or Right populations, and  
275 a choice-period input to the entire network (see Section 5.2.3). Here, we use EPI to determine the  
276 changes in network connectivity  $z = [sW_P, sW_A, vW_{PA}, vW_{AP}, dW_{PA}, dW_{AP}, hW_P, hW_A]$  resulting  
277 in greater levels of rapid task switching accuracy.

278 To quantify the emergent property of rapid task switching at various levels of accuracy, we consid-  
279 ered the requirements of this model in this behavioral paradigm. At the end of successful trials,  
280 the response of the Pro population in the hemisphere of the correct choice must have a value near  
281 1, while the Pro population in the opposite hemisphere must have a value near 0. Constraining a  
282 population response  $x_\alpha \in [0, 1]$  to be either 0 or 1 can be achieved by requiring that it has Bernoulli  
283 variance (see Section 5.2.3). Thus, we can formulate rapid task switching at a level of accuracy  
284  $p \in [0, 1]$  in both tasks in terms of the average steady response of the Pro population  $\hat{p}$  of the  
285 correct choice, the error in Bernoulli variance of that Pro neuron  $\sigma_{err}^2$ , and the average difference  
286 in Pro neuron responses  $d$  in both Pro and Anti trials:

$$\mathcal{B}(p) \triangleq \mathbb{E} \begin{bmatrix} \hat{p}_P \\ \hat{p}_A \\ (\hat{p}_P - p)^2 \\ (\hat{p}_A - p)^2 \\ \sigma_{P,err}^2 \\ \sigma_{A,err}^2 \\ d_P \\ d_A \end{bmatrix} = \begin{bmatrix} p \\ p \\ 0.15^2 \\ 0.15^2 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}. \quad (9)$$

287 Thus,  $\mathcal{B}(p)$  denotes Bernoulli, winner-take-all responses between Pro neurons in a model executing  
288 rapid task switching near accuracy level  $p$ .

289 We used EPI to learn distributions of the SC weight matrix parameters  $z$  conditioned on of various  
290 levels of rapid task switching accuracy  $\mathcal{B}(p)$  for  $p \in \{50\%, 60\%, 70\%, 80\%, 90\%\}$ . To make sense

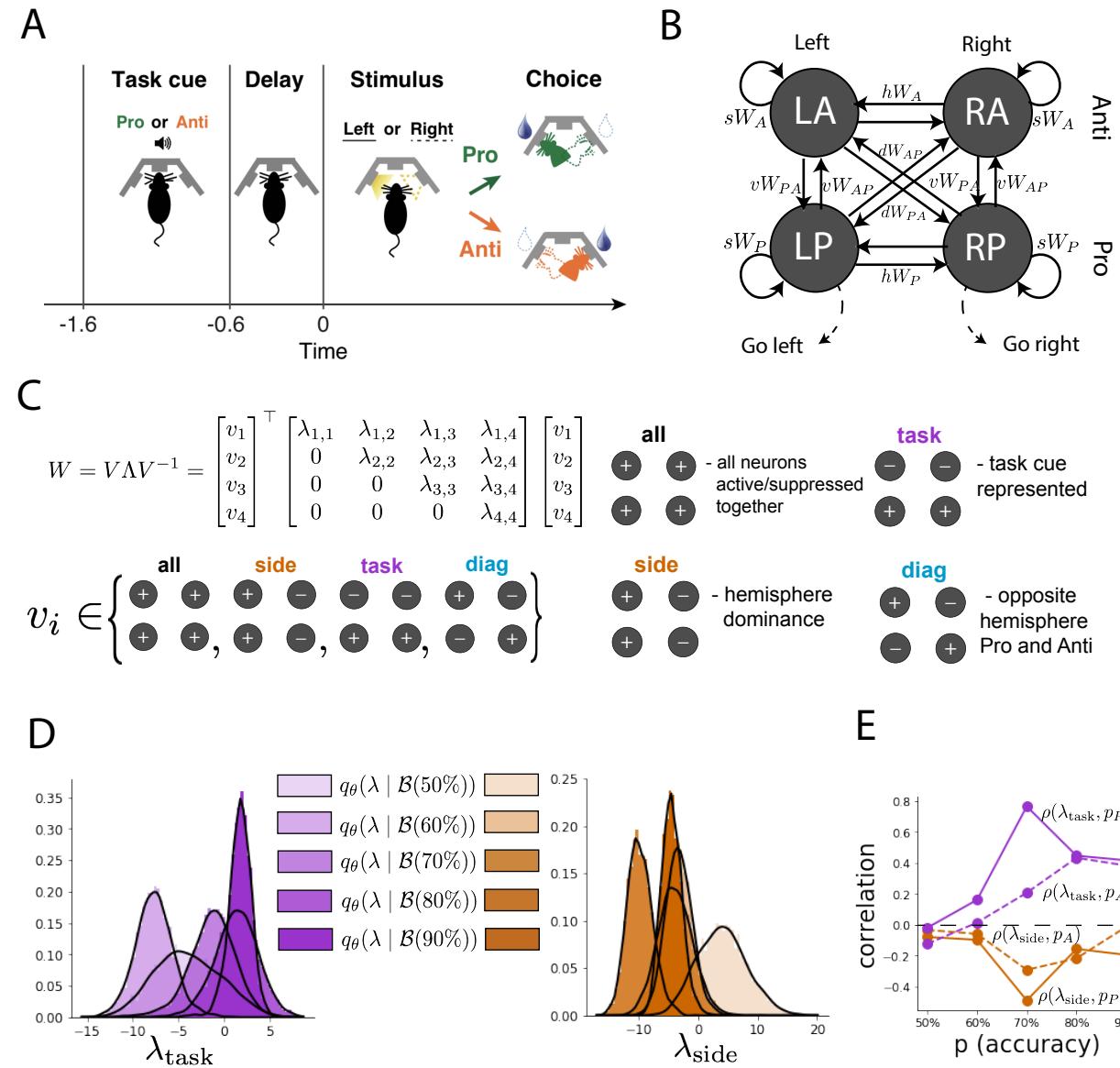


Figure 4: EPI reveals changes in SC [25] connectivity that control task accuracy. A. Rapid task switching behavioral paradigm (see text). B. Model of superior colliculus (SC). Neurons: LP - left pro, RP - right pro, LA - left anti, RA - right anti. Parameters:  $sW$  - self,  $hW$  - horizontal,  $vW$  - vertical,  $dW$  - diagonal weights. Subscripts  $P$  and  $A$  of connectivity weights indicate Pro or Anti populations, and e.g.  $vW_{PA}$  is a vertical weight from an Anti to a Pro population. C. The Schur decomposition of the weight matrix  $W = V \Lambda V^{-1}$  is a unique decomposition with orthogonal  $V$  and upper triangular  $\Lambda$ . Schur modes:  $v_{\text{all}}$ ,  $v_{\text{task}}$ ,  $v_{\text{side}}$ , and  $v_{\text{diag}}$ . 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.

of these inferred distributions, we followed the approach of Duan et al. by decomposing the connectivity matrix  $W = V\Lambda V^{-1}$  in such a way (the Schur decomposition) that the basis vectors  $v_i$  are the same for all  $W$  (Fig. 4C). These basis vectors have intuitive roles in processing for this task, and are accordingly named the *all* mode - all neurons co-fluctuate, *side* mode - one side dominates the other, *task* mode - the Pro or Anti populations dominate the other, and *diag* mode - Pro- and Anti-populations of opposite hemispheres dominate the opposite pair. The corresponding eigenvalues (e.g.  $\lambda_{\text{task}}$ , which change according to  $W$ ) indicate the degree to which activity along that mode is increased or decreased by  $W$ .

We found that for greater task accuracies, the task mode eigenvalue increases, indicating the importance of  $W$  to the task representation (Fig. 4D, purple; adjacent distributions from 60% to 90% have  $p < 10^{-4}$ , Mann-Whitney test with 50 estimates and 100 samples). Stepping from random chance (50%) networks to marginally task-performing (60%) networks, there is a marked decrease of the side mode eigenvalues (Fig. 4D, orange;  $p < 10^{-4}$ ). Such side mode suppression relative to 50% remains in the models achieving greater accuracy, revealing its importance towards task performance. There were no interesting trends with task accuracy in the all or diag mode (hence not shown in Fig. 4). Importantly, we can conclude from our methodology that side mode suppression in  $W$  allows rapid task switching, and that greater task-mode representations in  $W$  increase accuracy. These hypotheses are confirmed by forward simulation of the SC model (Fig. 4E, see Section 5.2.3) suggesting experimentally testable predictions: increase in rapid task switching performance should be correlated with changes in effective connectivity corresponding to an increase in task mode and decrease in side mode eigenvalues.

### 3.5 Linking RNN connectivity to error

So far, each model we have studied was designed from fundamental biophysical principles, genetically- or functionally-defined neuron types. At a more abstract level of modeling, recurrent neural networks (RNNs) are high-dimensional dynamical models of computation that are becoming increasingly popular in neuroscience research [49]. In theoretical neuroscience, RNN dynamics usually follow the equation

$$\frac{dx}{dt} = -x + W\phi(x) + h, \quad (10)$$

where  $x$  is the network activity,  $W$  is the network connectivity,  $\phi(\cdot) = \tanh(\cdot)$ , and  $h$  is the input to the system. Such RNNs are trained to do a task from a systems neuroscience experiment, and then the unit activations of the trained RNN are compared to recorded neural activity. Fully-connected

321 RNNs with tens of thousands of parameters are challenging to characterize [50], especially making  
 322 statistical inferences about their parameterization. Alternatively, we considered a rank-1,  $N$ -neuron  
 323 RNN with connectivity consisting of the sum of a random and a structured component:

$$W = g\chi + \frac{1}{N}mn^\top. \quad (11)$$

324 The random component  $g\chi$  has strength  $g$ , and random component weights are Gaussian dis-  
 325 tributed  $\chi_{i,j} \sim \mathcal{N}(0, \frac{1}{N})$ . The structured component  $\frac{1}{N}mn^\top$  has entries of  $m$  and  $n$  drawn from  
 326 Gaussian distributions  $m_i \sim \mathcal{N}(M_m, 1)$  and  $n_i \sim \mathcal{N}(M_n, 1)$ . Recent theoretical work derives the  
 327 low-dimensional response properties of low-rank networks from statistical parameterizations of their  
 328 connectivity, such as  $z = [g, M_m, M_n]$  [26]. We used EPI to infer the parameterizations of rank-  
 329 1 RNNs solving an example task, enabling discovery of properties of connectivity that result in  
 330 different types of error in the computation.

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

334 where:

$$\mu_{post} = \frac{\frac{\mu_0}{\sigma_0^2} + \frac{y}{\sigma_y^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma_y^2}} \quad \sigma_{post}^2 = \frac{1}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma_y^2}}. \quad (12)$$

335 To solve this Gaussian posterior conditioning task, the RNN response to a constant input  $h =$   
 336  $yr + (n - M_n)$  must equal the posterior mean along readout vector  $r$ , where

$$\kappa_r = \frac{1}{N} \sum_{j=1}^N r_j \phi(x_j). \quad (13)$$

337 Additionally, the amount of chaotic variance  $\Delta_T$  must equal the posterior variance. Theory for  
 338 low-rank RNNs allows us to express  $\kappa_r$  and  $\Delta_T$  in terms of each other through a solvable system of  
 339 nonlinear equations (see Section 5.2.4) [26]. This theory facilitates the mathematical formalization  
 340 of task execution into an emergent property, where the emergent property statistics of the RNN  
 341 activity are  $\kappa_r$  and  $\Delta_T$ , and the emergent property values are the ground truth posterior mean  
 342  $\mu_{post}$  and variance  $\sigma_{post}^2$ :

$$\mathbb{E} \begin{bmatrix} \kappa_r \\ \Delta_T \\ (\kappa_r - \mu_{post})^2 \\ (\Delta_T^2 - \sigma_{post}^2)^2 \end{bmatrix} = \begin{bmatrix} \mu_{post} \\ \sigma_{post}^2 \\ 0.1 \\ 0.1 \end{bmatrix}. \quad (14)$$

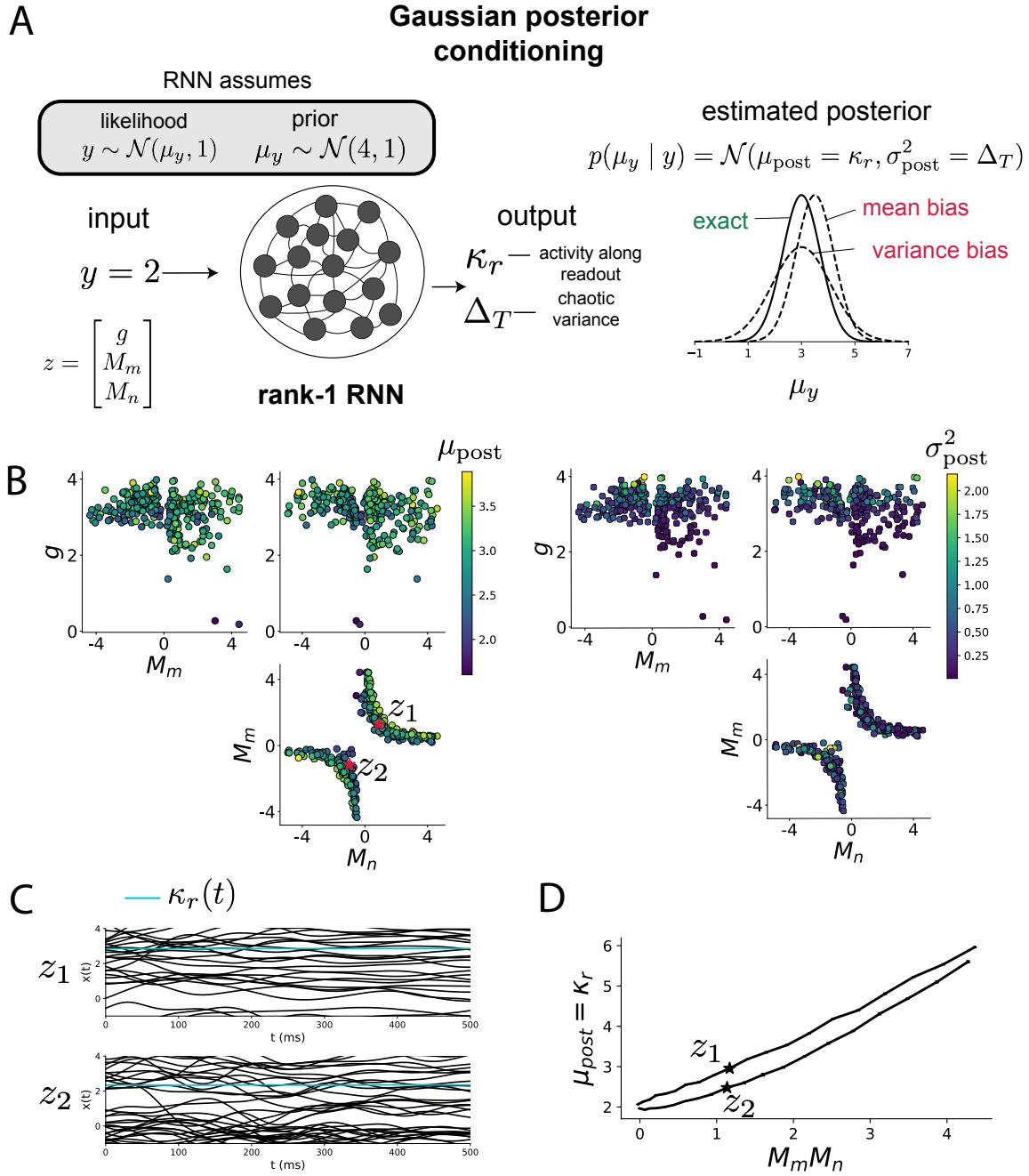


Figure 5: Sources of error in an RNN solving a simple task. A. (left) A rank-1 RNN executing a Gaussian posterior conditioning computation on  $\mu_y$ . (right) Error in this computation can come from over- or underestimating the posterior mean or variance. B. EPI distribution of rank-1 RNNs executing Gaussian posterior conditioning. Samples are colored by (left) posterior mean  $\mu_{\text{post}} = \kappa_r$  and (right) posterior variance  $\sigma_{\text{post}}^2 = \Delta_T$ . C. Finite-size network simulations of 2,000 neurons with parameters  $z_1$  and  $z_2$  sampled from the inferred distribution. Activity along readout  $\kappa_r$  (cyan) is stable despite chaotic fluctuations. D. The posterior mean computed by RNNs parameterized by  $z_1$  and  $z_2$  perturbed in the dimension of the product of  $M_m$  and  $M_n$ . Means and standard errors are shown across 10 realizations of 2,000-neuron networks.

343 We chose a substantial amount of variance in these emergent property statistics, so that the inferred  
 344 distribution resulted in RNNs with a variety of errors in their solutions to the gaussian posterior  
 345 conditioning problem.

346 EPI was used to learn distributions of RNN connectivity properties  $z = [g, M_m, M_n]$  executing  
 347 Gaussian posterior conditioning given an input of  $y = 2$ , where the true posterior is  $\mu_{\text{post}} = 3$  and  
 348  $\sigma_{\text{post}} = 0.5$  (Fig. 5A). We examined the nature of the over- and under-estimation of the posterior  
 349 means (Fig. 5B left) and variances (Fig. 5B right) in the inferred distributions (300 samples).  
 350 The symmetry in the  $M_m$ - $M_n$  plane, suggests a degeneracy in the product of  $M_m$  and  $M_n$  (Fig.  
 351 5B). Indeed,  $M_m M_n$  strongly determines the posterior mean ( $r = 0.62, p < 10^{-4}$ ). Furthermore,  
 352 the random strength  $g$  strongly determines the chaotic variance ( $r = 0.56, p < 10^{-4}$ ). Neither of  
 353 these observations were obvious from what mathematical analysis is available in networks of this  
 354 type (see Section 5.2.4). While the link between random strength  $g$  and chaotic variance  $\Delta_T$  (and  
 355 resultingly posterior variance in this problem) is well-known [3], the distribution admits a novel  
 356 hypothesis: the estimation of the posterior mean by the RNN increases with  $M_m M_n$ .

357 We tested this prediction by taking parameters  $z_1$  and  $z_2$  as representative samples from the positive  
 358 and negative  $M_m$ - $M_n$  quadrants, respectively. Instead of using the theoretical predictions shown in  
 359 Figure 5B, we simulated finite-size realizations of these networks with 2,000 neurons (e.g. Fig. 5C).  
 360 We perturbed these parameter choices by  $M_m M_n$  clarifying that the posterior mean can be directly  
 361 controlled in this way (Fig. 5D;  $p < 10^{-4}$ ), see Section 5.2.4). Thus, EPI confers a clear picture  
 362 of error in this computation: the product of the low rank vector means  $M_m$  and  $M_n$  modulates  
 363 the estimated posterior mean while the random strength  $g$  modulates the estimated posterior  
 364 variance. This novel procedure of inference on reduced parameterizations of RNNs conditioned on  
 365 the emergent property of task execution is generalizable to other settings modeled in [26] like noisy  
 366 integration and context-dependent decision making (Fig. S5).

## 367 4 Discussion

### 368 4.1 EPI is a general tool for theoretical neuroscience

369 Biologically realistic models of neural circuits are comprised of complex nonlinear differential equa-  
 370 tions, making traditional theoretical analysis and statistical inference intractable. We advance the  
 371 capabilities of statistical inference in theoretical neuroscience by presenting EPI, a deep inference  
 372 methodology for learning parameter distributions of theoretical models performing neural compu-

tation. We have demonstrated the utility of EPI 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 spiking frequency of membrane potentials, as well as high-level cognitive function like 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 applicability of EPI.

In this study, we have focused on applying EPI to low dimensional parameter spaces of models with low dimensional dynamical states. 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 produced state-of-the-art performance on high-dimensional tasks such as texture generation [20]. Of course, increasing the dimensionality of the dynamical state of the model makes optimization more expensive, and there is a practical limit there as with any machine learning approach. Although, theoretical approaches (e.g. [26]) can be used to reason about the wholistic activity of such high dimensional systems by introducing some degree of additional structure into the model.

There are additional technical considerations when assessing the suitability of EPI for a particular modeling question. First and foremost, as in any optimization problem, the defined emergent property should always be appropriately conditioned (constraints should not have wildly different units). Furthermore, if the program is underconstrained (not enough constraints), the distribution grows (in entropy) unstably unless mapped to a finite support. If overconstrained, there is no parameter set producing the emergent property, and EPI optimization will fail (appropriately). Next, one should consider the computational cost of the gradient calculations. In the best circumstance, there is a simple, closed form expression (e.g. Section 5.1.1) for the emergent property statistic given the model parameters. On the other end of the spectrum, many forward simulation iterations may be required before a high quality measurement of the emergent property statistic is available (e.g. Section 5.2.1). In such cases, optimization will be expensive.

## 4.2 Novel hypotheses from EPI

In neuroscience, machine learning has primarily been used to revealed structure in large-scale neural datasets [51, 52, 53, 54, 55, 56, 57] (see review, [15]). Such careful inference procedures are developed for these statistical models allowing precise, quantitative reasoning, which clarifies

404 the way data informs knowledge of the model parameters. However, these inferable statistical  
405 models lack resemblance to the underlying biology, making it unclear how to go from the structure  
406 revealed by these methods, to the neural mechanisms giving rise to it. In contrast, theoretical  
407 neuroscience has focused on careful mechanistic modeling and the production of emergent properties  
408 of computation. The careful steps of 1.) model design and 2.) emergent property definition, are  
409 followed by 3.) practical inference methods resulting in an opaque characterization of the way model  
410 parameters govern computation. In this work, we replaced this opaque procedure of parameter  
411 identification in theoretical neuroscience with emergent property inference, opening the door to  
412 careful inference in careful models of neural computation.

413 Biologically realistic models of neural circuits often prove formidable to analyze. Two main factors  
414 contribute to the difficulty of this endeavor. First, even in simple point-neuron circuit models,  
415 the number of parameters scales quadratically with the number of neurons, limiting the analytical  
416 dissection of its parameter space. Second, even in low dimensional circuits, the structure of the  
417 phase space itself is intricate and each parameter configuration can support multiple steady states  
418 [58] or non-trivial dynamics on strange attractors [59].

419 In Section 3.3, we advanced the tractability of low-dimensional neuronal circuit models by showing  
420 that EPI offers insights about cell-type specific input-responsivity that cannot be afforded through  
421 the available linear analytical methods [24, 44, 45]. By flexibly conditioning this V1 model on  
422 different emergent properties, we performed an exploratory analysis of a *model* rather than a  
423 dataset, generating a set of testable hypotheses, which were proved out. Furthermore, exploratory  
424 analyses can be directed towards formulating hypotheses of a specific form. For example, model  
425 parameter dependencies on behavioral performance can be assessed by using EPI to condition on  
426 various levels of task accuracy (See Section 3.4). This analysis identified experimentally testable  
427 predictions (proved out *in-silico*) of patterns of effective connectivity in SC that should be correlated  
428 with increased performance.

429 In our final analysis, we presented a novel procedure for doing statistical inference on interpretable  
430 parameterizations of RNNs executing simple tasks. Specifically, we analyzed RNNs solving a poste-  
431 rior conditioning problem in the spirit of [60]. This methodology relies on recently extended theory  
432 of responses in random neural networks with low-rank structure [26]. While we focused on rank-1  
433 RNNs, which were sufficient for solving this task, this inference procedure generalizes to RNNs  
434 of greater rank necessary for more complex tasks. The ability to apply the probabilistic model  
435 selection toolkit to RNNs should prove invaluable as their use in neuroscience increases.

436 EPI leverages deep learning technology for neuroscientific inquiry in a categorically different way  
437 than approaches focused on training neural networks to execute behavioral tasks [61]. This large  
438 body of research focused on examining optimized deep neural networks employs careful consid-  
439 eration of the objective function, learning rule, and architecture used. This endeavor efficiently  
440 obtains sets of parameters that can be reasoned about with respect to such considerations, but  
441 lacks the careful probabilistic treatment of parameter inference in EPI. These approaches can be  
442 used complementarily to enhance the practice of theoretical neuroscience.

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450 **Data availability statement:**

451 The datasets generated during and/or analysed during the current study are available from the  
452 corresponding author upon reasonable request.

453 **Code availability statement:**

454 The software written for the current study is available from the corresponding author upon rea-  
455 sonable request.

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632 **5 Methods**

633 **5.1 Emergent property inference (EPI)**

634 Emergent property inference (EPI) learns distributions of theoretical model parameters that pro-  
 635 duce emergent properties of interest by combining ideas from maximum entropy flow networks  
 636 (MEFNs) [20] and likelihood-free variational inference (LFVI) [21]. Consider model parameteri-  
 637 zation  $z$  and data  $x$  which has an intractable likelihood  $p(x | z)$  defined by a model simulator of  
 638 which samples are available  $x \sim p(x | z)$ . EPI optimizes a distribution  $q_\theta(z)$  (itself parameterized  
 639 by  $\theta$ ) of model parameters  $z$  to produce an emergent property of interest  $\mathcal{B}$ ,

$$\mathcal{B} \triangleq \mathbb{E}_{z \sim q_\theta} [\mathbb{E}_{x \sim p(x|z)} [T(x)]] = \mu. \quad (15)$$

640 Precisely, the emergent property statistics  $T(x)$  must equal the emergent property values  $\mu$ , in  
 641 expectation over the EPI distribution of parameters  $q_\theta(z)$  and the distribution of simulated activity  
 642  $p(x | z)$ . This is a viable way to represent emergent properties in theoretical models, as we have  
 643 demonstrated in the main text, and enables the EPI optimization.

644 With EPI, we use deep probability distributions to learn flexible approximations to model parameter  
 645 distributions  $q_\theta(z)$ . In deep probability distributions, a simple random variable  $w \sim q_0(w)$  is  
 646 mapped deterministically via a sequence of deep neural network layers ( $f_1, \dots, f_l$ ) parameterized by  
 647 weights and biases  $\theta$  to the support of the distribution of interest:

$$z = f_\theta(\omega) = f_l(\dots f_1(w)). \quad (16)$$

648 Given a simulator defined by a theoretical model  $x \sim p(x | z)$  and some emergent property of  
 649 interest  $\mathcal{B}$ ,  $q_\theta(z)$  is optimized via the neural network parameters  $\theta$  to find a maximally entropic  
 650 distribution  $q_\theta^*$  within the deep variational family  $\mathcal{Q}$  producing the emergent property:

$$\begin{aligned} q_\theta^*(z) &= \operatorname{argmax}_{q_\theta \in \mathcal{Q}} H(q_\theta(z)) \\ &\text{s.t. } \mathbb{E}_{z \sim q_\theta} [\mathbb{E}_{x \sim p(x|z)} [T(x)]] = \mu. \end{aligned} \quad (17)$$

651 Since we are optimizing parameters  $\theta$  of our deep probability distribution with respect to the  
 652 entropy  $H(q_\theta(z))$ , we must take gradients with respect to the log probability density of samples  
 653 from the deep probability distribution. Entropy of  $q_\theta(z)$  can be expressed as an expectation of  
 654 the negative log density of parameter samples  $z$  over the randomness in the parameterless initial  
 655 distribution  $q_0$ :

$$H(q_\theta(z)) = \int -q_\theta(z) \log(q_\theta(z)) dz = \mathbb{E}_{z \sim q_\theta} [-\log(q_\theta(z))] = \mathbb{E}_{w \sim q_0} [-\log(q_\theta(f_\theta(w)))]. \quad (18)$$

656 Thus, the gradient of the entropy of the deep probability distribution can be estimated as an  
 657 average of gradients of the log density of samples  $z$ :

$$\nabla_{\theta} H(q_{\theta}(z)) = \mathbb{E}_{w \sim q_0} [-\nabla_{\theta} \log(q_{\theta}(f_{\theta}(w)))]. \quad (19)$$

658 In EPI, MEFNs are purposed towards variational learning of model parameter distributions. A  
 659 closely related methodology, variational inference, uses optimization to approximate posterior dis-  
 660 tributions [62]. Standard methods like stochastic gradient variational Bayes [6] or black box varia-  
 661 tional inference [63] simply do not work for inference in theoretical models of neural circuits, since  
 662 they require tractable likelihoods  $p(x | z)$ . Work on likelihood-free variational inference (LFVI) [21],  
 663 which like EPI seeks to do inference in models with intractable likelihoods, employs an additional  
 664 deep neural network as a ratio estimator, enabling an estimation of the optimization objective for  
 665 variational inference. Like LFVI, EPI can be framed as variational inference (see Section 5.1.4).  
 666 But, unlike LFVI, EPI uses a single deep network to learn a distribution and is optimized to pro-  
 667 duce an emergent property, rather than condition on data points. Optimizing the EPI objective is  
 668 a technological challenge, the details of which we elaborate in Section 5.1.2. Before going through  
 669 those details, we ground this optimization in a toy example.

670 **5.1.1 Example: 2D LDS**

671 To gain intuition for EPI, consider a two-dimensional linear dynamical system (2D LDS) model  
 672 (Fig. S1A):

$$\tau \frac{dx}{dt} = Ax \quad (20)$$

673 with

$$A = \begin{bmatrix} a_1 & a_2 \\ a_3 & a_4 \end{bmatrix}. \quad (21)$$

674 To run EPI with the dynamics matrix elements as the free parameters  $z = [a_1, a_2, a_3, a_4]$  (fixing  
 675  $\tau = 1$ ), the emergent property statistics  $T(x)$  were chosen to contain the first and second moments  
 676 of the oscillatory frequency,  $2\pi\text{imag}(\lambda_1)$ , and the growth/decay factor,  $\text{real}(\lambda_1)$ , of the oscillating  
 677 system.  $\lambda_1$  is the eigenvalue of greatest real part when the imaginary component is zero, and  
 678 alternatively of positive imaginary component when the eigenvalues are complex conjugate pairs.  
 679 To learn the distribution of real entries of  $A$  that produce a band of oscillating systems around  
 680 1Hz, we formalized this emergent property as  $\text{real}(\lambda_1)$  having mean zero with variance  $0.25^2$ , and

681 the oscillation frequency  $2\pi\text{imag}(\lambda_1)$  having mean  $\omega = 1$  Hz with variance  $(0.1\text{Hz})^2$ :

$$\mathbb{E}[T(x)] \triangleq \mathbb{E} \begin{bmatrix} \text{real}(\lambda_1) \\ \text{imag}(\lambda_1) \\ (\text{real}(\lambda_1) - 0)^2 \\ (\text{imag}(\lambda_1) - 2\pi\omega)^2 \end{bmatrix} = \begin{bmatrix} 0.0 \\ 2\pi\omega \\ 0.25^2 \\ (2\pi\omega)^2 \end{bmatrix} \triangleq \mu. \quad (22)$$

682

683 Unlike the models we presented in the main text, this model admits an analytical form for the  
 684 mean emergent property statistics given parameter  $z$ , since the eigenvalues can be calculated using  
 685 the quadratic formula:

$$\lambda = \frac{\left(\frac{a_1+a_4}{\tau}\right) \pm \sqrt{\left(\frac{a_1+a_4}{\tau}\right)^2 + 4\left(\frac{a_2a_3-a_1a_4}{\tau}\right)}}{2}. \quad (23)$$

686 Importantly, even though  $\mathbb{E}_{x \sim p(x|z)}[T(x)]$  is calculable directly via a closed form function and  
 687 does not require simulation, we cannot derive the distribution  $q_\theta^*$  directly. This fact is due to the  
 688 formally hard problem of the backward mapping: finding the natural parameters  $\eta$  from the mean  
 689 parameters  $\mu$  of an exponential family distribution [64]. Instead, we used EPI to approximate this  
 690 distribution (Fig. S1B). We used a real-NVP normalizing flow architecture with four masks, two  
 691 neural network layers of 15 units per mask, with batch normalization momentum 0.99, mapped  
 692 onto a support of  $z_i \in [-10, 10]$ . (see Section 5.1.3).

693 Even this relatively simple system has nontrivial (though intuitively sensible) structure in the  
 694 parameter distribution. To validate our method, we analytically derived the contours of the prob-  
 695 ability density from the emergent property statistics and values. In the  $a_1$ - $a_4$  plane, the black  
 696 line at  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} = 0$ , dotted black line at the standard deviation  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} \pm 0.25$ ,  
 697 and the dotted gray line at twice the standard deviation  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} \pm 0.5$  follow the contour  
 698 of probability density of the samples (Fig. S2A). The distribution precisely reflects the desired  
 699 statistical constraints and model degeneracy in the sum of  $a_1$  and  $a_4$ . Intuitively, the parameters  
 700 equivalent with respect to emergent property statistic  $\text{real}(\lambda_1)$  have similar log densities.

701 To explain the bimodality of the EPI distribution, we examined the imaginary component of  $\lambda_1$ .

702 When  $\text{real}(\lambda_1) = \frac{a_1+a_4}{2} = 0$ , we have

$$\text{imag}(\lambda_1) = \begin{cases} \sqrt{\frac{a_1a_4-a_2a_3}{\tau}}, & \text{if } a_1a_4 < a_2a_3 \\ 0 & \text{otherwise} \end{cases}. \quad (24)$$

703 When  $\tau = 1$  and  $a_1a_4 > a_2a_3$  (center of distribution above), we have the following equation for the

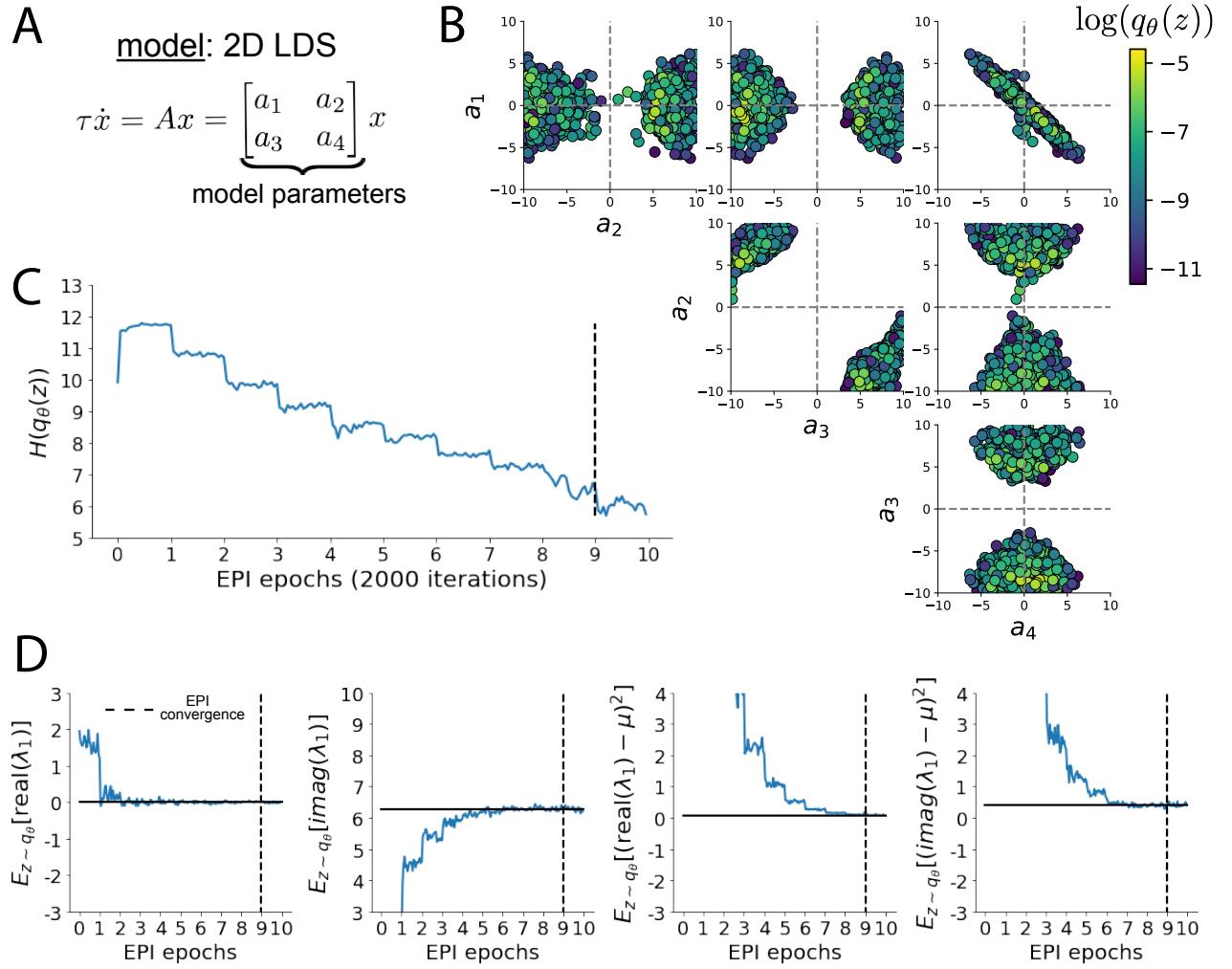


Fig. S1: A. Two-dimensional linear dynamical system model, where real entries of the dynamics matrix  $A$  are the parameters. B. The EPI distribution for a two-dimensional linear dynamical system with  $\tau = 1$  that produces an average of 1Hz oscillations with some small amount of variance. Dashed lines indicate the parameter axes. C. Entropy throughout the optimization. At the beginning of each augmented Lagrangian epoch (2,000 iterations), the entropy dipped 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 adjust closer to their constraints.

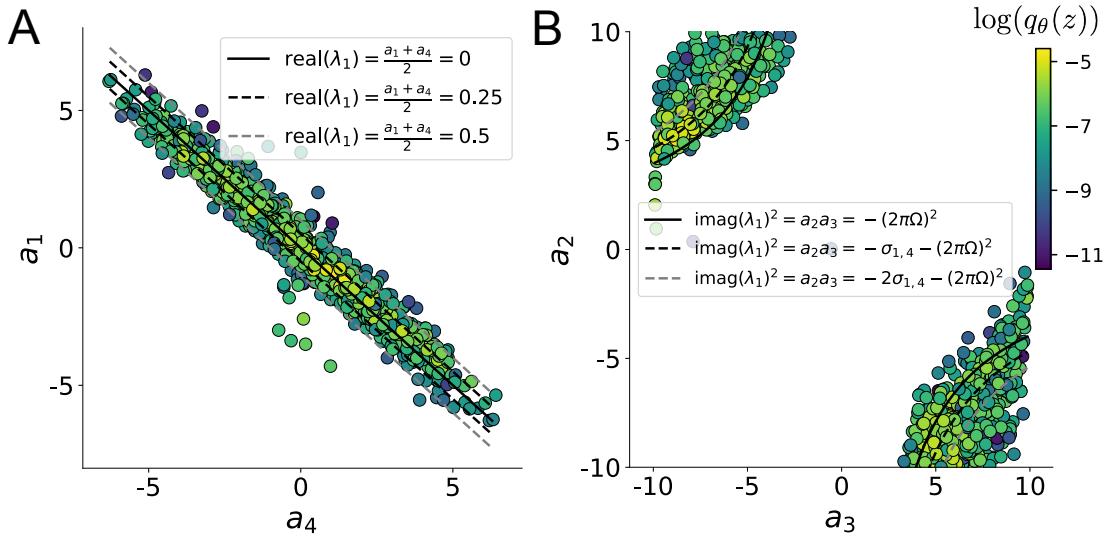


Fig. S2: A. Probability contours in the  $a_1$ - $a_4$  plane were derived from the relationship to emergent property statistic of growth/decay factor  $\text{real}(\lambda_1)$ . B. Probability contours in the  $a_2$ - $a_3$  plane were derived from the emergent property statistic of oscillation frequency  $2\pi\text{imag}(\lambda_1)$ .

704 other two dimensions:

$$\text{imag}(\lambda_1)^2 = a_1 a_4 - a_2 a_3 \quad (25)$$

705 Since we constrained  $\mathbb{E}_{z \sim q_\theta} [\text{imag}(\lambda)] = 2\pi$  (with  $\omega = 1$ ), we can plot contours of the equation  
 706  $\text{imag}(\lambda_1)^2 = a_1 a_4 - a_2 a_3 = (2\pi)^2$  for various  $a_1 a_4$  (Fig. S2B). With  $\sigma_{1,4} = \mathbb{E}_{z \sim q_\theta} (|a_1 a_4 - E_{q_\theta}[a_1 a_4]|)$ ,  
 707 we show the contours as  $a_1 a_4 = 0$  (black),  $a_1 a_4 = -\sigma_{1,4}$  (black dotted), and  $a_1 a_4 = -2\sigma_{1,4}$  (grey dotted). This validates the curved structure of the inferred distribution learned through EPI. We  
 708 took steps in negative standard deviation of  $a_1 a_4$  (dotted and gray lines), since there are few positive  
 709 values  $a_1 a_4$  in the learned distribution. Subtler combinations of model and emergent property will  
 710 have more complexity, further motivating the use of EPI for understanding these systems. As we  
 711 expect, the distribution results in samples of two-dimensional linear systems oscillating near 1Hz  
 712 (Fig. S3).

### 714 5.1.2 Augmented Lagrangian optimization

715 To optimize  $q_\theta(z)$  in Equation 17, the constrained optimization is executed using the augmented  
 716 Lagrangian method. The following objective is minimized:

$$L(\theta; \eta, c) = -H(q_\theta) + \eta^\top R(\theta) + \frac{c}{2} \|R(\theta)\|^2 \quad (26)$$

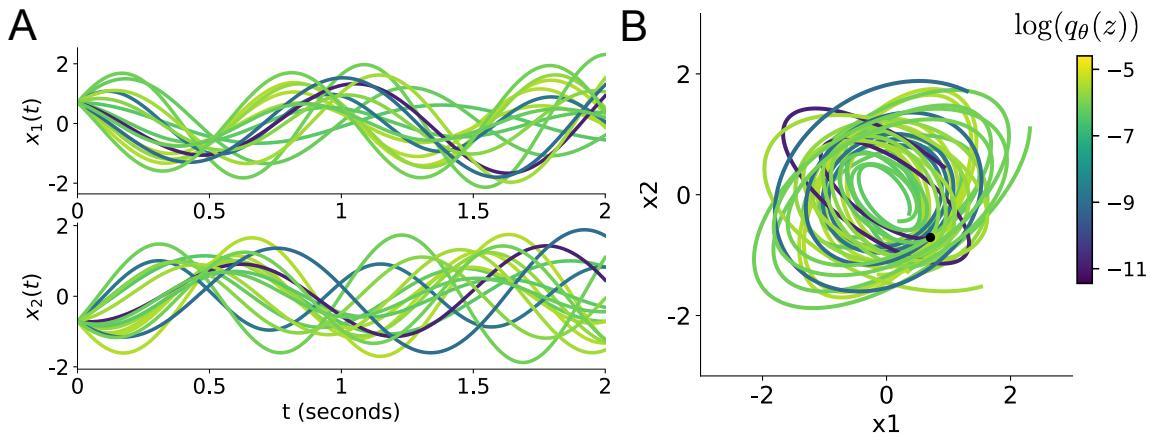


Fig. S3: Sampled dynamical systems  $z \sim q_\theta(z)$  and their simulated activity from  $x(0) = [\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}]$  colored by log probability. A. Each dimension of the simulated trajectories throughout time. B. The simulated trajectories in phase space.

717 where  $R(\theta) = \mathbb{E}_{z \sim q_\theta} [\mathbb{E}_{x \sim p(x|z)} [T(x) - \mu]]$ ,  $\eta \in \mathbb{R}^m$  are the Lagrange multipliers where  $m = |\mu| =$   
 718  $|T(x)|$ , and  $c$  is the penalty coefficient. These Lagrange multipliers are closely related to the natural  
 719 parameters of exponential families (see Section 5.1.4). Deep neural network weights and biases  $\theta$  of  
 720 the deep probability distribution are optimized according to Equation 26 using the Adam optimizer  
 721 with its standard parameterization [65].  $\eta$  is initialized to the zero vector and adapted following  
 722 each augmented Lagrangian epoch, which is a period of optimization with fixed  $(\eta, c)$  for a given  
 723 number of stochastic optimization iterations. A low value of  $c$  is used initially, and conditionally  
 724 increased after each epoch based on constraint error reduction. For example, the initial value of  
 725  $c$  was  $c_0 = 10^{-3}$  during EPI with the oscillating 2D LDS (Fig. S1C). The penalty coefficient is  
 726 updated based on the result of a hypothesis test regarding the reduction in constraint violation. The  
 727 p-value of  $\mathbb{E}[||R(\theta_{k+1})||] > \gamma \mathbb{E}[||R(\theta_k)||]$  is computed, and  $c_{k+1}$  is updated to  $\beta c_k$  with probability  
 728  $1 - p$ . The other update rule is  $\eta_{k+1} = \eta_k + c_k \frac{1}{n} \sum_{i=1}^n (T(x^{(i)}) - \mu)$  given a batch size  $n$ . Throughout  
 729 the study,  $\beta = 4.0$ ,  $\gamma = 0.25$ , and the batch size was a hyperparameter, which varied according to  
 730 the application of EPI.

731 The intention is that  $c$  and  $\eta$  start at values encouraging entropic growth early in optimization.  
 732 With each training epoch in which the update rule for  $c$  is invoked by unsatisfactory constraint  
 733 error reduction, the constraint satisfaction terms are increasingly weighted, resulting in a decreased  
 734 entropy. This encourages the discovery of suitable regions of parameter space, and the subsequent  
 735 refinement of the distribution to produce the emergent property. In the oscillating 2D LDS example,

736 each augmented Lagrangian epoch ran for 2,000 iterations (Fig. S1C-D). Notice the initial entropic  
 737 growth, and subsequent reduction upon each update of  $\eta$  and  $c$ . The momentum parameters of the  
 738 Adam optimizer were reset at the end of each augmented Lagrangian epoch.

739 Rather than starting optimization from some  $\theta$  drawn from a randomized distribution, we found  
 740 that initializing  $q_\theta(z)$  to approximate an isotropic Gaussian distribution conferred more stable, con-  
 741 sistent optimization. The parameters of the Gaussian initialization were chosen on an application-  
 742 specific basis. Throughout the study, we chose isotropic Gaussian initializations with mean  $\mu_{\text{init}}$  at  
 743 the center of the distribution support and some standard deviation  $\sigma_{\text{init}}$ , except for one case, where  
 744 an initialization informed by random search was used (see Section 5.2.2).

745 To assess whether EPI distribution  $q_\theta(z)$  produces the emergent property, we defined a hypothesis  
 746 testing convergence criteria. The algorithm has converged when a null hypothesis test of constraint  
 747 violations  $R(\theta)_i$  being zero is accepted for all constraints  $i \in \{1, \dots, m\}$  at a significance threshold  
 748  $\alpha = 0.05$ . This significance threshold is adjusted through Bonferroni correction according to the  
 749 number of constraints  $m$ . The p-values for each constraint are calculated according to a two-tailed  
 750 nonparametric test, where 200 estimations of the sample mean  $R(\theta)^i$  are made from  $k$  resamplings  
 751 of  $z$  from a finite sample of size  $n$  taken at the end of the augmented Lagrangian epoch.  $k$  is  
 752 determined by a fraction of the batch size  $\nu$ , which varies according to the application. In the  
 753 linear two-dimensional system example, we used a batch size of  $n = 1000$  and set  $\nu = 0.1$  resulting  
 754 in convergence after the ninth epoch of optimization. (Fig. S1C-D black dotted line).

### 755 5.1.3 Normalizing flows

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

$$q(z') = q(f^{-1}(z')) \left| \det \frac{\partial f^{-1}(z')}{\partial z'} \right| = q(z) \left| \det \frac{\partial f(z)}{\partial z} \right|^{-1}. \quad (27)$$

759 However, this computation has cubic complexity in dimensionality for fully connected layers. By  
 760 restricting our layers to normalizing flows [17] – bijective functions with fast log determinant Ja-  
 761 cobian computations, we can tractably optimize deep generative models with objectives that are a  
 762 function of sample density, like entropy. Most of our analyses use either a planar flow [17] or real  
 763 NVP [66], which have proven effective in our architecture searches. Planar flow architectures are

764 specified by the number of planar bijection layers used, while real NVP architectures are specified  
 765 by the number of masks, neural network layers per mask, units per layer, and batch normalization  
 766 momentum parameter.

767 **5.1.4 Emergent property inference as variational inference in an exponential family**

768 Now that we have fully described the EPI method, we consider its broader contextualization as a  
 769 statistical method and its relation to Bayesian inference. In Bayesian inference a prior belief about  
 770 model parameters  $z$  is formalized into a prior distribution  $p(z)$ , and the statistical model capturing  
 771 the effect of  $z$  on observed data points  $x$  is formalized in the likelihood distribution  $p(x | z)$ . In  
 772 Bayesian inference, we obtain a posterior distribution  $p(z | x)$ , which captures how the data inform  
 773 our knowledge of model parameters using Bayes' rule:

$$p(z | x) = \frac{p(x | z)p(z)}{p(x)}. \quad (28)$$

774 The posterior distribution is analytically available when the prior is conjugate with the likelihood.  
 775 However, conjugacy is rare in practice, and alternative methods, such as variational inference [62],  
 776 are utilized.

777 As we compare EPI to variational inference, it is important to consider that EPI is a maximum  
 778 entropy method, and that maximum entropy methods have a fundamental relationship with expo-  
 779 nential family distributions. A maximum entropy distribution of form:

$$\begin{aligned} p^*(z) &= \underset{p \in \mathcal{P}}{\operatorname{argmax}} H(p(z)) \\ \text{s.t. } \mathbb{E}_{z \sim p}[T(z)] &= \mu. \end{aligned} \quad (29)$$

780 will have probability density in the exponential family:

$$p^*(z) \propto \exp(\eta^\top T(z)). \quad (30)$$

781 The mappings between the mean parameterization  $\mu$  and the natural parameterization  $\eta$  are for-  
 782 mally hard to identify [64].

783 Now, consider the goal of doing variational inference with an exponential family posterior dis-  
 784 tribution  $p(z | x)$ . We use the following abbreviated notation to collect the base measure  $b(z)$   
 785 and sufficient statistics  $T(z)$  into  $\tilde{T}(z)$  and likewise concatenate a 1 onto the end of the natural

786 parameter  $\tilde{\eta}(x)$ . The log normalizing constant  $A(\eta(x))$  remains unchanged:

$$\begin{aligned} p(z | x) &= b(z) \exp \left( \eta(x)^\top T(z) - A(\eta(x)) \right) = \exp \left( \begin{bmatrix} \eta(x) \\ 1 \end{bmatrix}^\top \begin{bmatrix} T(z) \\ b(z) \end{bmatrix} - A(\eta(x)) \right). \\ &= \exp \left( \tilde{\eta}(x)^\top \tilde{T}(z) - A(\eta(x)) \right) \end{aligned} \quad (31)$$

787 Variational inference with an exponential family posterior distribution uses optimization to mini-  
788 mize the following divergence [62]:

$$q_\theta^* = \operatorname{argmin}_{q_\theta \in Q} KL(q_\theta || p(z | x)). \quad (32)$$

789  $q_\theta(z)$  is the variational approximation to the posterior with variational parameters  $\theta$ . We can write  
790 this KL divergence in terms of entropy of the variational approximation:

$$KL(q_\theta || p(z | x)) = \mathbb{E}_{z \sim q_\theta} [\log(q_\theta(z))] - \mathbb{E}_{z \sim q_\theta} [\log(p(z | x))] \quad (33)$$

791

$$= -H(q_\theta) - \mathbb{E}_{z \sim q_\theta} \left[ \tilde{\eta}(x)^\top \tilde{T}(z) - A(\eta(x)) \right]. \quad (34)$$

792 As far as the variational optimization is concerned, the log normalizing constant is independent of  
793  $q_\theta(z)$ , so it can be dropped

$$\operatorname{argmin}_{q_\theta \in Q} KL(q_\theta || p(z | x)) = \operatorname{argmin}_{q_\theta \in Q} -H(q_\theta) - \mathbb{E}_{z \sim q_\theta} \left[ \tilde{\eta}(x)^\top \tilde{T}(z) \right]. \quad (35)$$

794 Further, we can write the objective in terms of the first moment of the sufficient statistics  $\mu =$   
795  $\mathbb{E}_{z \sim p(z|x)} [T(z)]$ :

$$= \operatorname{argmin}_{q_\theta \in Q} -H(q_\theta) - \mathbb{E}_{z \sim q_\theta} \left[ \tilde{\eta}(x)^\top (\tilde{T}(z) - \mu) \right] + \tilde{\eta}(x)^\top \mu, \quad (36)$$

796 which simplifies to

$$= \operatorname{argmin}_{q_\theta \in Q} -H(q_\theta) - \mathbb{E}_{z \sim q_\theta} \left[ \tilde{\eta}(x)^\top (\tilde{T}(z) - \mu) \right]. \quad (37)$$

797 .

798 In comparison, in emergent property inference (EPI), we solve the following problem:

$$q_\theta^*(z) = \operatorname{argmax}_{q_\theta \in Q} H(q_\theta(z)), \text{ s.t. } \mathbb{E}_{z \sim q_\theta} [\mathbb{E}_{x \sim p(x|z)} [T(x)]] = \mu. \quad (38)$$

799 The Lagrangian objective (without augmentation) is

$$q_\theta^* = \operatorname{argmin}_{q_\theta \in Q} -H(q_\theta) + \eta_{\text{opt}}^\top \left( \mathbb{E}_{z \sim q_\theta} [\tilde{T}(z)] - \mu \right). \quad (39)$$

800 Thus, as the optimization proceeds,  $\eta_{\text{opt}}^\top$  should converge to the natural parameter  $\tilde{\eta}(x)$  through  
801 its adaptations in each epoch (see Section 5.1.2).

We have shown that there is indeed a clear relationship between Bayesian inference and EPI. Specifically, EPI is executing variational inference in an exponential family posterior, whose sufficient statistics are the emergent property statistics and mean parameterization are the emergent property values. However, in EPI we have not specified a prior distribution, or collected data, which can inform us about model parameters. Instead we have a mathematical specification of an emergent property, which the model must produce, and a maximum entropy selection principle. Accordingly, we replace the notation of  $p(z | x)$  with  $p(z | \mathcal{B})$  conceptualizing an inferred distribution that obeys emergent property  $\mathcal{B}$  (see Section 5.1).

## 5.2 Theoretical models

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

### 5.2.1 Stomatogastric ganglion

We analyze how the parameters  $z = [g_{el}, g_{synA}]$  govern the emergent phenomena of network syncing in a model of the stomatogastric ganglion (STG) [23] shown in Figure 1A with activity  $x = [x_{f1}, x_{f2}, x_{hub}, x_{s1}, x_{s2}]$ , using the same hyperparameter choices as Gutierrez et al. Each neuron's membrane potential  $x_\alpha(t)$  for  $\alpha \in \{f1, f2, hub, s1, s2\}$  is the solution of the following differential equation:

$$C_m \frac{dx_\alpha}{dt} = -[h_{leak}(x; z) + h_{Ca}(x; z) + h_K(x; z) + h_{hyp}(x; z) + h_{elec}(x; z) + h_{syn}(x; z)]. \quad (40)$$

The membrane potential of each neuron is affected by the leak, calcium, potassium, hyperpolarization, electrical and synaptic currents, respectively, which are functions of all membrane potentials and the conductance parameters  $z$ . The capacitance of the cell membrane was set to  $C_m = 1nF$ . Specifically, the currents are the difference in the neuron's membrane potential and that current type's reversal potential multiplied by a conductance:

$$h_{leak}(x; z) = g_{leak}(x_\alpha - V_{leak}) \quad (41)$$

$$h_{elec}(x; z) = g_{el}(x_\alpha^{post} - x_\alpha^{pre}) \quad (42)$$

$$h_{syn}(x; z) = g_{syn}S_\infty^{pre}(x_\alpha^{post} - V_{syn}) \quad (43)$$

$$h_{Ca}(x; z) = g_{Ca}M_\infty(x_\alpha - V_{Ca}) \quad (44)$$

827

828

$$h_K(x; z) = g_K N(x_\alpha - V_K) \quad (45)$$

$$h_{hyp}(x; z) = g_h H(x_\alpha - V_{hyp}). \quad (46)$$

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

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

$$M_\infty = 0.5 \left( 1 + \tanh \left( \frac{x_\alpha - v_1}{v_2} \right) \right) \quad (47)$$

837

$$\frac{dN}{dt} = \lambda_N(N_\infty - N) \quad (48)$$

838

$$N_\infty = 0.5 \left( 1 + \tanh \left( \frac{x_\alpha - v_3}{v_4} \right) \right) \quad (49)$$

839

$$\lambda_N = \phi_N \cosh \left( \frac{x_\alpha - v_3}{2v_4} \right) \quad (50)$$

840

$$\frac{dH}{dt} = \frac{(H_\infty - H)}{\tau_h} \quad (51)$$

841

$$H_\infty = \frac{1}{1 + \exp \left( \frac{x_\alpha + v_5}{v_6} \right)} \quad (52)$$

842

$$\tau_h = 272 - \left( \frac{-1499}{1 + \exp \left( \frac{-x_\alpha + v_7}{v_8} \right)} \right). \quad (53)$$

843 where we set  $v_1 = 0mV$ ,  $v_2 = 20mV$ ,  $v_3 = 0mV$ ,  $v_4 = 15mV$ ,  $v_5 = 78.3mV$ ,  $v_6 = 10.5mV$ ,  
 844  $v_7 = -42.2mV$ ,  $v_8 = 87.3mV$ ,  $v_9 = 5mV$ , and  $v_{th} = -25mV$ .

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

$$S_\infty = \frac{1}{1 + \exp \left( \frac{v_{th} - x_\alpha}{v_9} \right)}. \quad (54)$$

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

848 In order to measure the frequency of the hub neuron during EPI, the STG model was simulated  
 849 for  $T = 200$  time steps of  $dt = 25ms$ . In EPI, since gradients are taken through the simulation  
 850 process, the number of time steps are kept modest if possible. The chosen  $dt$  and  $T$  were the  
 851 most computationally convenient choices yielding accurate frequency measurement. Poor resolution  
 852 afforded by the discrete Fourier transform motivated the use of an alternative basis of complex  
 853 exponentials to measure spiking frequency. Instead, we used a basis of complex exponentials with  
 854 frequencies from 0.0-1.0 Hz at 0.01Hz resolution,  $\Phi = [0.0, 0.01, \dots, 1.0]^\top$

855 Another consideration was that the frequency spectra of the neuron membrane potentials had sev-  
 856 eral peaks. High-frequency sub-threshold activity obscured the maximum frequency measurement  
 857 in the complex exponential basis. Accordingly, subthreshold activity was set to zero, and the  
 858 whole signal was low-pass filtered with a moving average window of length 20. The signal was  
 859 subsequently mean centered. After this preprocessing, the maximum frequency in the filter bank  
 860 accurately reflected the firing frequency.

861 Finally, to differentiate through the maximum frequency identification, we used a sum-of-powers  
 862 normalization. Let  $\mathcal{X}_\alpha \in \mathcal{C}^{|\Phi|}$  be the complex exponential filter bank dot products with the signal  
 863  $x_\alpha \in \mathbb{R}^N$ , where  $\alpha \in \{\text{f1}, \text{f2}, \text{hub}, \text{s1}, \text{s2}\}$ . The “frequency identification” vector is

$$v_\alpha = \frac{|\mathcal{X}_\alpha|^\beta}{\sum_{k=1}^N |\mathcal{X}_\alpha(k)|^\beta}. \quad (55)$$

864 The frequency is then calculated as  $\omega_\alpha = v_\alpha^\top \Phi$  with  $\beta = 100$ .

865 Network syncing, like all other emergent properties in this work, are defined by the emergent  
 866 property statistics and values. The emergent property statistics are the first and second moments  
 867 of the firing frequencies. The first moments were set to 0.53Hz, and the second moments were set  
 868 to 0.025Hz<sup>2</sup>:

$$E \begin{bmatrix} \omega_{\text{f1}} \\ \omega_{\text{f2}} \\ \omega_{\text{hub}} \\ \omega_{\text{s1}} \\ \omega_{\text{s2}} \\ (\omega_{\text{f1}} - 0.53)^2 \\ (\omega_{\text{f2}} - 0.53)^2 \\ (\omega_{\text{hub}} - 0.53)^2 \\ (\omega_{\text{s1}} - 0.53)^2 \\ (\omega_{\text{s2}} - 0.53)^2 \end{bmatrix} = \begin{bmatrix} 0.53 \\ 0.53 \\ 0.53 \\ 0.53 \\ 0.53 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \end{bmatrix} \quad (56)$$

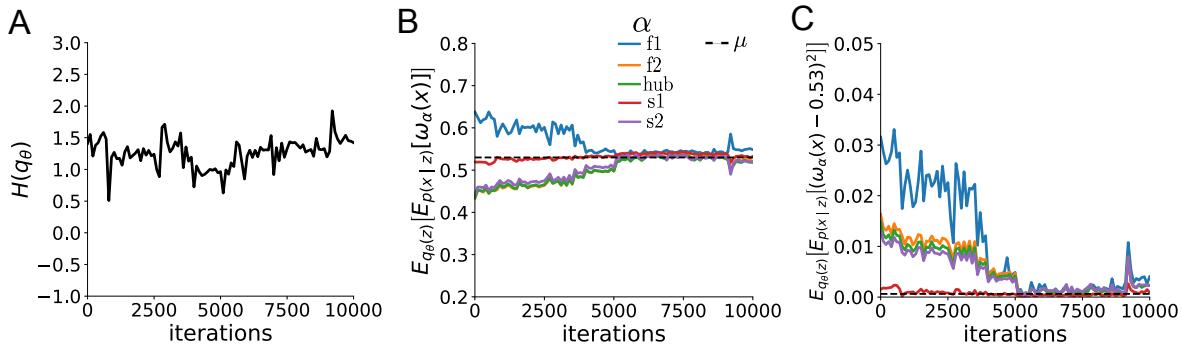


Fig. S4: EPI optimization of the STG model producing network syncing. A. Entropy throughout optimization. B. The first moment emergent property statistics converge to the emergent property values at 10,000 iterations, following the fourth augmented Lagrangian epoch of 2,500 iterations. Since  $q_\theta(z)$  failed to produce enough samples yielding  $\omega_{f1}(x)$  less than 0.53Hz, the convergence criteria were not satisfied after the third epoch at 7,500 iterations. C. The second moment emergent property statistics converge to the emergent property values.

869 for the EPI distribution shown in Fig. 1B. Throughout optimization, the augmented Lagrangian  
 870 parameters  $\eta$  and  $c$ , were updated after each epoch of 2,500 iterations (see Section 5.1.2). The  
 871 optimization converged after four epochs (Fig. S4).

872 For EPI in Fig 2C, we used a real NVP architecture with four masks and two layers of 10 units  
 873 per mask, and batch normalization momentum of 0.99 mapped onto a support of  $z = [g_{el}, g_{synA}] \in$   
 874  $[4, 8] \times [0, 4]$ . We used an augmented Lagrangian coefficient of  $c_0 = 10^2$ , a batch size  $n = 300$ ,  
 875 set  $\nu = 0.1$ , and initialized  $q_\theta(z)$  to produce an isotropic Gaussian with mean  $\mu_{\text{init}} = [6, 2]$  with  
 876 standard deviation  $\sigma_{\text{init}} = 0.5$ .

877 We calculated the Hessian at the mode of the inferred EPI distribution. The Hessian of a probability  
 878 model is the second order gradient of the log probability density  $\log q_\theta(z)$  with respect to the  
 879 parameters  $z$ :  $\frac{\partial^2 \log q_\theta(z)}{\partial z \partial z^\top}$ . With EPI, we can examine the Hessian, which is analytically available  
 880 throughout distribution, to indicate the dimensions of parameter space that are sensitive (high  
 881 magnitude eigenvalue), and which are degenerate (low magnitude eigenvalue) with respect to the  
 882 emergent property produced. In Figure 1B, the eigenvectors of the Hessian  $v_1$  and  $v_2$  are shown  
 883 evaluated at the mode of the distribution. The length of the arrows is inversely proportional to the  
 884 square root of absolute value of their eigenvalues  $\lambda_1 = -10.8$  and  $\lambda_2 = -2.27$ . We quantitatively  
 885 measured the sensitivity of the model with respect to network syncing along the eigenvectors of the  
 886 Hessian (Fig. 1B, inset). Sensitivity was measured as the slope coefficient of linear regression fit

887 to network syncing error (the sum of squared differences of each neuron's frequency from 0.53Hz)  
 888 as a function of parametric perturbation magnitude (maximum 0.25) away from the mode along  
 889 both orientations indicated by the eigenvector with 100 equally spaced samples. The sensitivity  
 890 slope coefficient of eigenvector  $v_1$  with respect to network syncing was significant ( $\beta = 4.82 \times 10^{-2}$ ,  
 891  $p < 10^{-4}$ ). In contrast, eigenvector  $v_2$  did not identify a dimension of parameter space significantly  
 892 sensitive to network syncing ( $\beta = 8.65 \times 10^{-4}$  with  $p = .67$ ). These sensitivities were compared to  
 893 all other dimensions of parameter space (100 equally spaced angles from 0 to  $\pi$ ), revealing that the  
 894 Hessian eigenvectors indeed identified the directions of greatest sensitivity and degeneracy (Fig.  
 895 1B, inset). The contours of Figure 1 were calculated as error in  $T(x)$  from  $\mu$  in both the first and  
 896 second moment emergent property statistics.

897 **5.2.2 Primary visual cortex**

898 The dynamics of each neural populations average rate  $x = [x_E, x_P, x_S, x_V]^\top$  are given by:

$$899 \quad \tau \frac{dx}{dt} = -x + [Wx + h]_+^n. \quad (57)$$

900 By consolidating information from many experimental datasets, Billeh et al. [47] produce estimates  
 of the synaptic strength (in mV)

$$901 \quad M = \begin{bmatrix} 0.36 & 0.48 & 0.31 & 0.28 \\ 1.49 & 0.68 & 0.50 & 0.18 \\ 0.86 & 0.42 & 0.15 & 0.32 \\ 1.31 & 0.41 & 0.52 & 0.37 \end{bmatrix} \quad (58)$$

902 and connection probability

$$903 \quad C = \begin{bmatrix} 0.16 & 0.411 & 0.424 & 0.087 \\ 0.395 & .451 & 0.857 & 0.02 \\ 0.182 & 0.03 & 0.082 & 0.625 \\ 0.105 & 0.22 & 0.77 & 0.028 \end{bmatrix}. \quad (59)$$

904 Multiplying these connection probabilities and synaptic efficacies gives us an effective connectivity  
 matrix:

$$905 \quad W_{\text{full}} = C \odot M = \begin{bmatrix} 0.16 & 0.411 & 0.424 & 0.087 \\ 0.395 & .451 & 0.857 & 0.02 \\ 0.182 & 0.03 & 0.082 & 0.625 \\ 0.105 & 0.22 & 0.77 & 0.028 \end{bmatrix}. \quad (60)$$

904 Theoretical work on these systems considers a subset of the effective connectivities [24, 44, 45]

$$W = \begin{bmatrix} W_{EE} & W_{EP} & W_{ES} & 0 \\ W_{PE} & W_{PP} & W_{PS} & 0 \\ W_{SE} & 0 & 0 & W_{SV} \\ W_{VE} & W_{VP} & W_{VS} & 0 \end{bmatrix}. \quad (61)$$

905 In coherence with this work, we only keep the entries of  $W_{\text{full}}$  corresponding to parameters in  
906 Equation 61.

907 We look at how this four-dimensional nonlinear dynamical model of V1 responds to different inputs,  
908 and compare the predictions of the linear response to the approximate posteriors obtained through  
909 EPI. The input to the system is the sum of a baseline input  $b = [1, 1, 1, 1]^\top$  and a differential input  
910  $dh$ :

$$h = b + dh. \quad (62)$$

911 All simulations of this system had  $T = 100$  time points, a time step  $dt = 5\text{ms}$ , and time constant  
912  $\tau = 20\text{ms}$ . The system was initialized to a random draw  $x(0)_i \sim \mathcal{N}(1, 0.01)$ .

913 We can describe the dynamics of this system more generally by

$$\dot{x}_i = -x_i + f(u_i) \quad (63)$$

914 where the input to each neuron is

$$u_i = \sum_j W_{ij}x_j + h_i. \quad (64)$$

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

$$\frac{dx_{ss}}{dh} = F(W \frac{dx_{ss}}{dh} + I) \quad (65)$$

916 which is calculable by

$$\frac{dx_{ss}}{dh} = (F^{-1} - W)^{-1}. \quad (66)$$

917 This calculation is used to produce the magenta lines in Figure 2C, which show the linearly predicted  
918 inputs that generate a response from two standard deviations (of  $\mathcal{B}$ ) below and above  $y$ .

919 The emergent property we considered was the first and second moments of the change in steady  
920 state rate  $dx_{ss}$  between the baseline input  $h = b$  and  $h = b + dh$ . We use the following notation to  
921 indicate that the emergent property statistics were set to the following values:

$$\mathcal{B}(\alpha, y) \triangleq \mathbb{E} \begin{bmatrix} dx_{\alpha,ss} \\ (dx_{\alpha,ss} - y)^2 \end{bmatrix} = \begin{bmatrix} y \\ 0.01^2 \end{bmatrix}. \quad (67)$$

922 In the final analysis for this model, we sweep the input one neuron at a time away from the mode  
 923 of each inferred distributions  $dh^* = z^* = \operatorname{argmax}_z \log q_\theta(z \mid \mathcal{B}(\alpha, 0.1))$ . The differential responses  
 924  $\delta x_{\alpha,ss}$  are examined at perturbed inputs  $h = b + dh^* + \delta h_\alpha \hat{u}_\alpha$  where  $\hat{u}_\alpha$  is a unit vector in the  
 925 dimension of  $\alpha$  and  $\delta x$  is evaluated at 101 equally spaced samples of  $\delta h_\alpha$  from -15 to 15.

926 We measured the linear regression slope between neuron-types of  $\delta x$  and  $\delta h$  to confirm the hy-  
 927 potheses H1-H3 (H4 is simply observing the nonmonotonicity) and report the p values for tests of  
 928 non-zero slope.

929 H1: the neuron-type responses are sensitive to their direct inputs. E-population:  $\beta = 1.62$ ,  
 930  $p < 10^{-4}$  (Fig. 3A black), P-population:  $\beta = 1.06$ ,  $p < 10^{-4}$  (Fig. 3B blue), S-population:  
 931  $\beta = 6.80$ ,  $p < 10^{-4}$  (Fig. 3C red), V-population:  $\beta = 6.41$ ,  $p < 10^{-4}$  (Fig. 3D green).

932 H2: the E-population ( $\beta = 0$ ,  $p = 1$ ) and P-populations ( $\beta = 0$ ,  $p = 1$ ) are not affected by  
 933  $\delta h_V$  (Fig. 3A green, 3B green);

934 H3: the S-population is not affected by  $\delta h_P$  ( $\beta = 0$ ,  $p = 1$ ) (Fig. 3C blue);

935

936 For each  $\mathcal{B}(\alpha, y)$  with  $\alpha \in \{E, P, S, V\}$  and  $y \in \{0.1, 0.5\}$ , we ran EPI using a real NVP architecture  
 937 of four masks layers with two hidden layers of 10 units, mapped to a support of  $z_i \in [-5, 5]$  with  
 938 no batch normalization. We used an augmented Lagrangian coefficient of  $c_0 = 10^5$ , a batch size  
 939  $n = 1000$ , set  $\nu = 0.5$ . The EPI distributions shown in Fig. 2 are the converged distributions with  
 940 maximum entropy across random seeds.

941 We set the parameters of the Gaussian initialization  $\mu_{\text{init}}$  and  $\Sigma_{\text{init}}$  to the mean and covariance of  
 942 random samples  $z^{(i)} \sim \mathcal{U}(-5, 5)$  that produced emergent property statistic  $dx_{\alpha,ss}$  within a bound  
 943  $\epsilon$  of the emergent property value  $y$ .  $\epsilon = 0.01$  was set to be one standard deviation of the emergent  
 944 property value according to the emergent property value  $0.01^2$  of the variance emergent property  
 945 statistic.

### 946 5.2.3 Superior colliculus

947 In the model of Duan et al [25], there are four total units: two in each hemisphere corresponding to  
 948 the Pro/Contra and Anti/Ipsi populations. They are denoted as left Pro (LP), left Anti (LA), right  
 949 Pro (RP) and right Anti (RA). Each unit has an activity ( $x_\alpha$ ) and internal variable ( $u_\alpha$ ) related  
 950 by

$$x_\alpha = \left( \frac{1}{2} \tanh \left( \frac{u_\alpha - \epsilon}{\zeta} \right) + \frac{1}{2} \right) \quad (68)$$

951 where  $\alpha \in \{LP, LA, RA, RP\}$   $\epsilon = 0.05$  and  $\zeta = 0.5$  control the position and shape of the nonlin-  
 952 earity, respectively.

953 We order the elements of  $x$  and  $u$  in the following manner

$$x = \begin{bmatrix} x_{LP} \\ x_{LA} \\ x_{RP} \\ x_{RA} \end{bmatrix} \quad u = \begin{bmatrix} u_{LP} \\ u_{LA} \\ u_{RP} \\ u_{RA} \end{bmatrix}. \quad (69)$$

954 The internal variables follow dynamics:

$$\tau \frac{du}{dt} = -u + Wx + h + \sigma dB \quad (70)$$

955 with time constant  $\tau = 0.09s$  and Gaussian noise  $\sigma dB$  controlled by the magnitude of  $\sigma = 1.0$ . The  
 956 weight matrix has 8 parameters  $sW_P$ ,  $sW_A$ ,  $vW_{PA}$ ,  $vW_{AP}$ ,  $hW_P$ ,  $hW_A$ ,  $dW_{PA}$ , and  $dW_{AP}$  (Fig.  
 957 4B):

$$W = \begin{bmatrix} sW_P & vW_{PA} & hW_P & dW_{PA} \\ vW_{AP} & sW_A & dW_{AP} & hW_A \\ hW_P & dW_{PA} & sW_P & vW_{PA} \\ dW_{AP} & hW_A & vW_{AP} & sW_A \end{bmatrix}. \quad (71)$$

958 The system receives five inputs throughout each trial, which has a total length of 1.8s.

$$h = h_{\text{rule}} + h_{\text{choice-period}} + h_{\text{light}}. \quad (72)$$

959 There are rule-based inputs depending on the condition,

$$h_{P,\text{rule}}(t) = \begin{cases} I_{P,\text{rule}}[1, 0, 1, 0]^\top, & \text{if } t \leq 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (73)$$

$$h_{A,\text{rule}}(t) = \begin{cases} I_{A,\text{rule}}[0, 1, 0, 1]^\top, & \text{if } t \leq 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (74)$$

960 a choice-period input,

$$h_{\text{choice}}(t) = \begin{cases} I_{\text{choice}}[1, 1, 1, 1]^\top, & \text{if } t > 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (75)$$

and an input to the right or left-side depending on where the light stimulus is delivered.

$$h_{\text{light}}(t) = \begin{cases} I_{\text{light}}[1, 1, 0, 0]^\top, & \text{if } t > 1.2s \text{ and Left} \\ I_{\text{light}}[0, 0, 1, 1]^\top, & \text{if } t > 1.2s \text{ and Right} \\ 0, & t \leq 1.2s \end{cases} \quad (76)$$

The input parameterization was fixed to  $I_{P,\text{rule}} = 10$ ,  $I_{A,\text{rule}} = 10$ ,  $I_{\text{choice}} = 2$ , and  $I_{\text{light}} = 1$ .

To produce an accuracy rate of  $p_{LP}$  in the Left, Pro condition, let  $\hat{p}_i$  be the empirical average steady state response (final  $x_{LP}$  at end of task) over M=500 Gaussian noise draws for a given SC model parameterization  $z_i$ :

$$\hat{p}_i = \mathbb{E}_{\sigma dB} [x_{LP} | s = L, c = P, z = z_i] = \frac{1}{M} \sum_{j=1}^M x_{LP}(s = L, c = P, z = z_i, \sigma dB_j) \quad (77)$$

where stimulus  $s \in \{L, R\}$ , cue  $c \in \{P, A\}$ , and  $\sigma dB_j$  is the Gaussian noise on trial  $j$ . As with the V1 model, we only consider steady state responses of  $x$ , so  $x_\alpha$  is used from here on to denote the steady state activity at the end of the trial. For the first emergent property statistic, the average over EPI samples (from  $q_\theta(z)$ ) is set to the desired value  $p_{LP}$ :

$$\mathbb{E}_{z_i \sim q_\phi} [\mathbb{E}_{\sigma dB} [x_{LP,ss} | s = L, c = P, z = z_i]] = \mathbb{E}_{z_i \sim q_\phi} [\hat{p}_i] = p_{LP}. \quad (78)$$

For the next emergent property statistic, we ask that the variance of the steady state responses across Gaussian draws, is the Bernoulli variance for the empirical rate  $\hat{p}_i$ :

$$\mathbb{E}_{z \sim q_\phi} [\sigma_{err}^2] = 0 \quad (79)$$

where the Bernoulli variance error  $\sigma_{err}^2$  for the Pro task, left condition is

$$\sigma_{err}^2 = Var_{\sigma dB} [x_{LP} | s = L, c = P, z = z_i] - \hat{p}_i(1 - \hat{p}_i). \quad (80)$$

We have an additional constraint that the Pro neuron on the opposite hemisphere should have the opposite value (0 and 1). We can enforce this with another constraint:

$$\mathbb{E}_{z \sim q_\phi} [d_P] = 1, \quad (81)$$

where the distance between Pro neuron steady states  $d_P$  in the Pro condition is

$$d_P = \mathbb{E}_{\sigma dB} [(x_{LP} - x_{RP})^2 | s = L, c = P, z = z_i] \quad (82)$$

977 The emergent property statistics only need to be measured during the Left stimulus condition of  
 978 the Pro and Anti tasks, since the network is symmetrically parameterized. In total, the emergent  
 979 property of rapid task switching at accuracy level  $p$  was defined as

$$\mathcal{B}(p) \triangleq \mathbb{E} \begin{bmatrix} \hat{p}_P \\ \hat{p}_A \\ (\hat{p}_P - p)^2 \\ (\hat{p}_A - p)^2 \\ \sigma_{P,err}^2 \\ \sigma_{A,err}^2 \\ d_P \\ d_A \end{bmatrix} = \begin{bmatrix} p \\ p \\ 0.15^2 \\ 0.15^2 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}. \quad (83)$$

980 Since the maximum variance of a random variable bounded from 0 to 1 is the Bernoulli variance  
 981  $\hat{p}(1 - \hat{p})$ , and the maximum squared difference between two variables bounded from 0 to 1 is 1, we  
 982 do not need to control the second moment of these test statistics. These variables are dynamical  
 983 system states and can only exponentially decay (or saturate) to 0 (or 1), so the Bernoulli variance  
 984 error and squared difference constraints cannot be satisfied exactly in simulation. This is important  
 985 to be mindful of when evaluating the convergence criteria. Instead of using our usual hypothesis  
 986 testing criteria for convergence to the emergent property, we set a slack variable threshold only for  
 987 these technically infeasible emergent property values to 0.05.

988 Using EPI to learn distributions of dynamical systems producing Bernoulli responses at a given rate  
 989 (with small variance around that rate) was more challenging than expected. There is a pathology in  
 990 this optimization setup, where the learned distribution of weights is bimodal attributing a fraction  
 991  $p$  of the samples to an expansive mode (which always sends  $x_{LP}$  to 1), and a fraction  $1 - p$  to a  
 992 decaying mode (which always sends  $x_{LP}$  to 0). This pathology was avoided using an inequality  
 993 constraint prohibiting parameter samples that resulted in low variance of responses across noise.

994 For each accuracy level  $p$ , we ran EPI for 10 different random seeds using an architecture of 10  
 995 planar flows with a support of  $z \in \mathbb{R}^8$ . We used an augmented Lagrangian coefficient of  $c_0 = 10^2$ , a  
 996 batch size  $n = 300$ , and set  $\nu = 0.5$ , and initialized  $q_\theta(z)$  to produce an isotropic Gaussian of zero  
 997 mean with standard deviation  $\sigma_{\text{init}} = 1$ . The EPI distributions shown in Fig. 4 are the converged  
 998 distributions with maximum entropy across random seeds.

999 We report significant correlations  $r$  and their p-values from Figure 4E in Table 1. Correlations were  
 1000 measured from 5,000 samples of  $q_\theta(z | \mathcal{B}(p))$  and p-values are reported for one-tailed tests, since

$\lambda$	$\hat{p}$	$q_\theta(z)$	$r$	p-value
$\lambda_{\text{task}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(60\%))$	$1.24 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{task}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(70\%))$	$7.56 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{task}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(80\%))$	$4.59 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{task}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(90\%))$	$3.76 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{task}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(60\%))$	$4.80 \times 10^{-02}$	$p < .01$
$\lambda_{\text{task}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(70\%))$	$2.08 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{task}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(80\%))$	$4.84 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{task}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(90\%))$	$4.25 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(50\%))$	$-7.57 \times 10^{-02}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(60\%))$	$-6.73 \times 10^{-02}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(70\%))$	$-4.86 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(80\%))$	$-1.43 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_P$	$q(z \mid \mathcal{B}(90\%))$	$-1.93 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(60\%))$	$-7.60 \times 10^{-02}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(70\%))$	$-2.73 \times 10^{-01}$	$p < 10^{-4}$
$\lambda_{\text{side}}$	$\hat{p}_A$	$q(z \mid \mathcal{B}(80\%))$	$-2.74 \times 10^{-01}$	$p < 10^{-4}$

Table 1: Table of significant correlation values from Fig. 4E.

1001 we hypothesized a positive correlation between task accuracies  $p_P$  or  $p_A$  and  $\lambda_{\text{task}}$ , and a negative  
 1002 correlation between task accuracies  $p_P$  and  $p_A$  and  $\lambda_{\text{side}}$ .

1003 **5.2.4 Rank-1 RNN**

1004 Extensive research on random fully-connected recurrent neural networks has resulted in founda-  
 1005 tional theories of their activity [3, 67]. Furthermore, independent research on training these models  
 1006 to perform computations suggests that learning occurs through low-rank perturbations to the con-  
 1007 nectivity (e.g. [68, 69]). Recent theoretical work extends theory for random neural networks [3]  
 1008 to those with added low-rank structure [26]. In Section 3.5, we used this theory to enable EPI on  
 1009 RNN parameters conditioned on the emergent property of task execution.

1010 Such RNNs have the following dynamics:

$$\frac{dx}{dt} = -x + W\phi(x) + h, \quad (84)$$

1011 where  $x$  is network activity,  $W$  is the connectivity weight matrix,  $\phi(\cdot) = \tanh(\cdot)$  is the input-output  
 1012 function, and  $h$  is the input to the system. In a rank-1 RNN (which was sufficiently complex for  
 1013 the Gaussian posterior conditioning task),  $W$  is the sum of a random component with strength  $g$   
 1014 and a structured component determined by the outer product of vectors  $m$  and  $n$ :

$$W = g\chi + \frac{1}{N}mn^\top, \quad (85)$$

1015 where  $\chi_{ij} \sim \mathcal{N}(0, \frac{1}{N})$ , and the entries of  $m$  and  $n$  are distributed as  $m_i \sim \mathcal{N}(M_m, 1)$  and  
 1016  $n_i \sim \mathcal{N}(M_n, 1)$ . For EPI, we consider  $z = [g, M_m, M_n]$ , which are the parameters governing  
 1017 the connectivity properties of the RNN.

1018 From such a parameterization  $z$ , the theory of Mastrogiovise et al. produces solutions for variables  
 1019 describing the low dimensional response properties of the RNN. These “dynamic mean field” (DMF)  
 1020 variables (e.g. the activity along a vector  $\kappa_v$ , the total variance  $\Delta_0$ , structured variance  $\Delta_\infty$ , and  
 1021 the chaotic variance  $\Delta_T$ ) are derived to be functions of one another and connectivity parameters  
 1022  $z$ . The collection of these derived functions results in a system of equations, whose solution must  
 1023 be obtained through a nonlinear system of equations solver. The iterative steps of this system  
 1024 of equations solver are differentiable, so we take gradients through this solve process. The DMF  
 1025 variables provide task-relevant information about the RNN’s response to task inputs.

1026 In the Gaussian posterior conditioning example,  $\kappa_r$  and  $\Delta_T$  are DMF variables used as task-relevant  
 1027 emergent property statistics  $\mu_{\text{post}}$  and  $\sigma_{\text{post}}^2$ . Specifically, we solve for the DMF variables  $\kappa_r$ ,  $\kappa_n$ ,  
 1028  $\Delta_0$  and  $\Delta_\infty$ , where the readout is nominally chosen to point in the unit orthant  $r = [1, \dots, 1]^\top$ . The  
 1029 consistency equations for these variables in the presence of a constant input  $h = yr - (n - M_n)$  can  
 1030 be derived following [26]:

$$\begin{aligned} \kappa_r &= G_1(\kappa_r, \kappa_n, \Delta_0, \Delta_\infty) = M_m \kappa_n + y \\ \kappa_n &= G_2(\kappa_r, \kappa_n, \Delta_0, \Delta_\infty) = M_n \langle [\phi_i] \rangle + \langle [\phi'_i] \rangle \\ \frac{\Delta_0^2 - \Delta_\infty^2}{2} &= G_3(\kappa_r, \kappa_n, \Delta_0, \Delta_\infty) = g^2 \left( \int \mathcal{D}z \Phi^2(\kappa_r + \sqrt{\Delta_0} z) - \int \mathcal{D}z \int \mathcal{D}x \Phi(\kappa_r + \sqrt{\Delta_0 - \Delta_\infty} x + \sqrt{\Delta_\infty} z) \right) \\ &\quad + (\kappa_n^2 + 1)(\Delta_0 - \Delta_\infty) \\ \Delta_\infty &= G_4(\kappa_r, \kappa_n, \Delta_0, \Delta_\infty) = g^2 \int \mathcal{D}z \left[ \int \mathcal{D}x \phi(\kappa_r + \sqrt{\Delta_0 - \Delta_\infty} x + \sqrt{\Delta_\infty} z) \right]^2 + \kappa_n^2 + 1 \end{aligned} \quad (86)$$

1031 where here  $z$  is a gaussian integration variable. We can solve these equations by simulating the  
 1032 following Langevin dynamical system to a steady state:

$$\begin{aligned}
l(t) &= \frac{\Delta_0(t)^2 - \Delta_\infty(t)^2}{2} \\
\Delta_0(t) &= \sqrt{2l(t) + \Delta_\infty(t)^2} \\
\frac{d\kappa_r(t)}{dt} &= -\kappa_r(t) + G_1(\kappa_r(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \\
\frac{d\kappa_n(t)}{dt} &= -\kappa_n + G_2(\kappa_r(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \\
\frac{dl(t)}{dt} &= -l(t) + G_3(\kappa_r(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t)) \\
\frac{d\Delta_\infty(t)}{dt} &= -\Delta_\infty(t) + G_4(\kappa_r(t), \kappa_n(t), \Delta_0(t), \Delta_\infty(t))
\end{aligned} \tag{87}$$

1033 Then, the chaotic variance, which is necessary for the Gaussian posterior conditioning example, is  
1034 simply calculated via  $\Delta_T = \Delta_0 - \Delta_\infty$ .

1035 We ran EPI using a real NVP architecture of two masks and two layers per mask with 10 units  
1036 mapped to a support of  $z = [g, M_m, M_n] \in [0, 5] \times [-5, 5] \times [-5, 5]$  with no batch normalization.  
1037 We used an augmented Lagrangian coefficient of  $c_0 = 1$ , a batch size  $n = 300$ , set  $\nu = 0.15$ ,  
1038 and initialized  $q_\theta(z)$  to produce an isotropic Gaussian with mean  $\mu_{\text{init}} = [2.5, 0, 0]$  with standard  
1039 deviation  $\sigma_{\text{init}} = 2.0$ . The EPI distribution shown in Fig. 5 is the converged distributions with  
1040 maximum entropy across five random seeds.

1041 To examine the effect of product  $M_m M_n$  on the posterior mean,  $\mu_{\text{post}}$  we took perturbations in  
1042  $M_m M_n$  away from two representative parameters  $z_1$  and  $z_2$  in 21 equally space increments from  
1043 -1 to 1. For each perturbation, we sampled 10 2,000-neuron RNNs and measure the calculated  
1044 posterior means. In Fig. 5D, we plot the product of  $M_m M_n$  in the perturbation versus the average  
1045 posterior mean across 10 network realizations with standard error bars. The correlation between  
1046 perturbation product  $M_m M_n$  and  $\mu_{\text{post}}$  was measured over all simulations. For perturbations away  
1047 from  $z_1$  the correlation was 0.995 with  $p < 10^{-4}$ , and for perturbations away from  $z_2$  the correlation  
1048 was 0.983 with  $p < 10^{-4}$ .

1049 In addition to the Gaussian posterior conditioning example in Section 3.5, we modeled two tasks  
1050 from Mastrogiovisepp et al.: noisy detection and context-dependent discrimination. We used the  
1051 same theoretical equations and task setups described in their study.

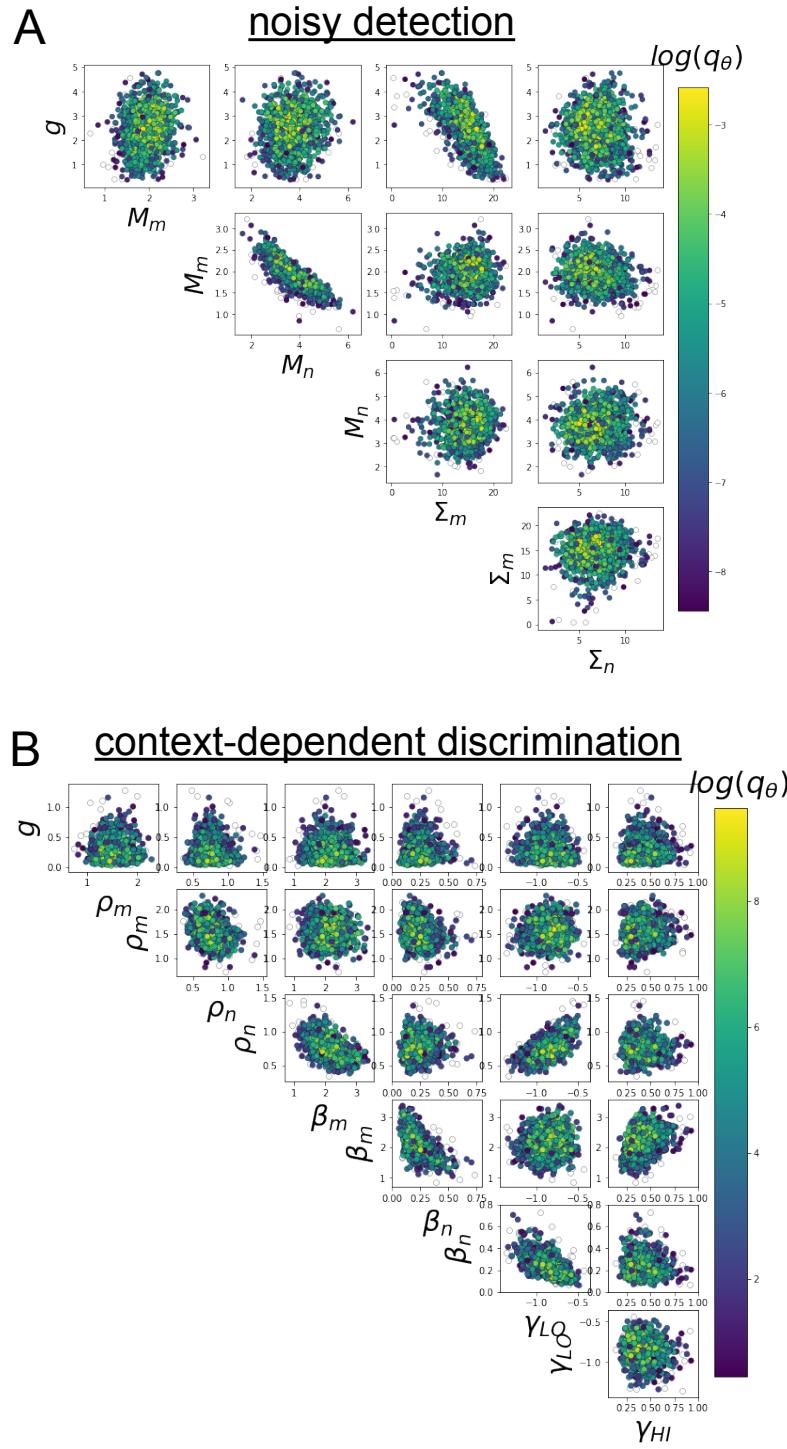


Fig. S5: A. EPI for rank-1 networks doing noisy discrimination. B. EPI for rank-2 networks doing context-dependent discrimination. See [26] for theoretical equations and task description.