

# Interrogating theoretical models of neural computation with deep inference

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

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

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

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

27 when configured appropriately, give rise to a measurable signature of a computation. The work of  
28 analyzing a model then becomes the inverse problem: given a computation of interest, how can we  
29 reason about these suitable parameter configurations – their likely values, their uniquenesses and  
30 degeneracies, their attractor states and phase transitions, and more?

31 Consider the idealized practice: a theorist considers a model carefully and analytically derives how  
32 model parameters govern the computation. Seminal examples of this gold standard include our  
33 field’s understanding of memory capacity in associative neural networks [2], chaos and autocorrela-  
34 tion timescales in random neural networks [3], and the paradoxical effect in excitatory/inhibitory  
35 networks [4]. Unfortunately, as circuit models include more biological realism, theory via analytic  
36 derivation becomes intractable. This fact creates an unfavorable tradeoff for the theorist. On the  
37 one hand, one may tractably analyze systems of equations with unrealistic assumptions (for ex-  
38 ample symmetry or gaussianity), producing accurate inferences about parameters of a too-simple  
39 model. On the other hand, one may choose a more biologically relevant model at the cost of *ad hoc*  
40 approaches to analysis (simply examining simulated activity), producing questionable or partial  
41 inferences about parameters of an appropriately complex, scientifically relevant model.

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

55 However, these inference tools have not significantly influenced the study of theoretical neuroscience  
56 models, for at least three reasons. First, at a practical level, the nonlinearities and dynamics of  
57 many theoretical models are such that conventional inference tools typically produce a narrow  
58 set of insights into these models. Indeed, only in the last few years has deep learning research

59 advanced to a point of relevance to this class of problem. Second, the object of interest from a  
60 theoretical model is not typically data itself, but rather a qualitative phenomenon – inspection of  
61 model behavior, or better, a measurable signature of some computation – an *emergent property* of  
62 the model. Third, because theoreticians work carefully to construct a model that has biological  
63 relevance, such a model as a result often does not fit cleanly into the framing of a statistical model.  
64 Technically, because many such models stipulate a noisy system of differential equations that can  
65 only be sampled or realized through forward simulation, they lack the explicit likelihood and priors  
66 central to the probabilistic modeling toolkit.

67 To address these three challenges, we developed an inference methodology – ‘emergent property  
68 inference’ – which learns a distribution over parameter configurations in a theoretical model. Crit-  
69 ically, this distribution is such that draws from the distribution (parameter configurations) corre-  
70 spond to systems of equations that give rise to a specified emergent property. First, we stipulate a  
71 bijective deep neural network that induces a flexible family of probability distributions over model  
72 parameterizations with a probability density we can calculate [15, 16, 17]. Second, we quantify  
73 the notion of emergent properties as a set of moment constraints on datasets generated by the  
74 model. Thus, an emergent property is not a single data realization, but a phenomenon or a feature  
75 of the model, which is ultimately the object of interest to the theorist (compared to the statisti-  
76 cal neuroscientist). Conditioning on an emergent property requires a variant of deep probabilistic  
77 inference methods, which we have previously introduced [18]. Third, because we cannot assume  
78 the theoretical model has explicit likelihood on data or the emergent property of interest, we use  
79 stochastic gradient techniques in the spirit of likelihood free variational inference [19]. Taken to-  
80 gether, emergent property inference (EPI) provides a methodology for inferring and then reasoning  
81 about parameter configurations that give rise to particular emergent phenomena in theoretical  
82 models. To clarify the technical details of EPI, we use it to analyze network syncing in a classic  
83 model of the stomatogastric ganglion [20].

84 Equipped with this methodology, we then investigated three models of current importance in theo-  
85 retical neuroscience. These models were chosen to demonstrate generality through ranges of biolog-  
86 ical realism (conductance-based biophysics to recurrent neural networks), neural system function  
87 (pattern generation to abstract cognitive function), and network scale (four to infinite neurons).  
88 First, we use EPI to produce a set of verifiable hypotheses of input-responsivity in a four neuron-  
89 type dynamical model of primary visual cortex; we then validate these hypotheses in the model.  
90 Second, we demonstrated how the systematic application of EPI to levels of task performance can

91 generate experimentally testable hypotheses regarding connectivity in superior colliculus. Third,  
 92 we use EPI to uncover the sources of bias in a low-rank recurrent neural network executing a toy  
 93 mathematical computation. The novel scientific insights offered by EPI contextualize and clarify  
 94 the previous studies exploring these models [20, 21, 22, 23] and more generally, suggests a depar-  
 95 ture from realism vs tractability considerations towards the use of modern machine learning for  
 96 sophisticated interrogation of biologically relevant models.

97 We note that, during our preparation and early presentation of this work [24, 25], another work  
 98 has arisen with broadly similar goals: bringing statistical inference to mechanistic models of neural  
 99 circuits [26]. We are excited by this broad problem being recognized by the community, and we  
 100 emphasize that these works offer complementary neuroscientific contributions and use different  
 101 technical methodologies. Scientifically, our work has focused primarily on systems-level theoretical  
 102 models, while their focus has been on lower-level cellular models. Secondly, there are several key  
 103 technical differences in the approaches (see Section A.1.4) perhaps most notably is our focus on  
 104 the emergent property – the measurable signal of the computation in question, vs their focus  
 105 on observed datasets; both certainly are worthy pursuits. The existence of these complementary  
 106 methodologies emphasizes the increased importance and timeliness of both works.

## 107 3 Results

### 108 3.1 Motivating emergent property inference of theoretical models

109 Consideration of the typical workflow of theoretical modeling clarifies the need for emergent prop-  
 110 erty inference. First, the theorist designs or chooses an existing model that, it is hypothesized,  
 111 captures the computation of interest. To ground this process in a well-known example, consider  
 112 the stomatogastric ganglion (STG) of crustaceans, a small neural circuit which generates multiple  
 113 rhythmic muscle activation patterns for digestion [27]. Despite full knowledge of STG connectivity  
 114 and a precise characterization of its rhythmic pattern generation, biophysical models of the STG  
 115 have complicated relationships between circuit parameters and neural activity [?]. A model of the  
 116 STG [20] 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  
 119 faster frequency than the mutually inhibiting slow neurons ( $s_1$  and  $s_2$ ), and the hub neuron (hub)  
 120 couples with the fast or slow population or both.

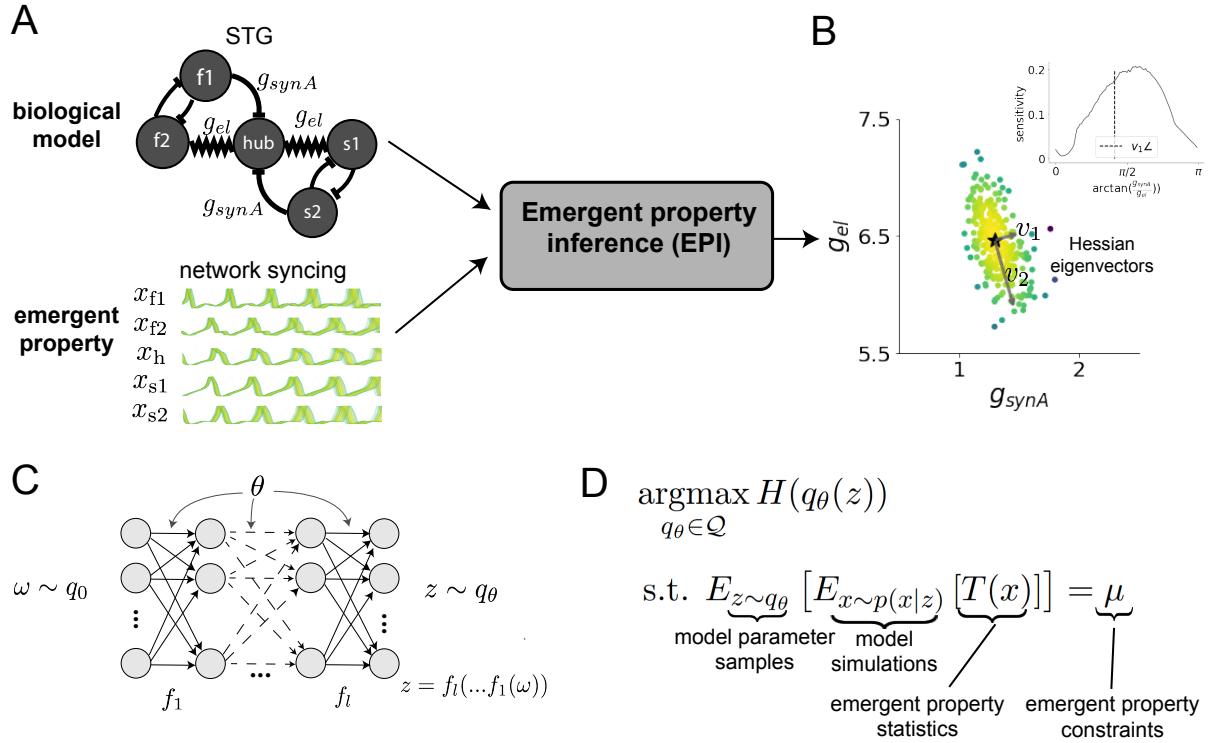


Figure 1: Emergent property inference (EPI) in the stomatogastric ganglion. A. For a choice of model (STG) and emergent property (network syncing), emergent property inference (EPI) learns a posterior distribution of the model parameters  $z = [g_{\text{el}}, g_{\text{synA}}]^T$  conditioned on network syncing. B. An EPI distribution of STG model parameters producing network syncing. The eigenvectors of the Hessian at the mode of the inferred distribution are indicated as  $v_1$  and  $v_2$ . (Inset) Sensitivity of the system with respect to network syncing along all dimensions of parameter space away from the mode. (see Section A.2.1). C. Deep probability distributions map a latent random variable  $\omega \sim q_0$ , where  $q_0$  is chosen to be simple distribution such as an isotropic gaussian, through a highly expressive function family  $f_\theta(\omega) = f_l(\dots f_1(\omega))$  parameterized by the neural network weights and biases  $\theta \in \Theta$ . This mapping induces an implicit probability model  $q(g_\theta(\omega)) \in \mathcal{Q}$  D. EPI learns a distribution  $q_\theta(z)$  of model parameters that produce an emergent property: the emergent property statistics  $T(x)$  are fixed in expectation over parameter distribution samples  $z \sim q_\theta(z)$  to particular values  $\mu$ . EPI distributions maximize randomness via entropy, although other measures are sensible.

121 Second, once the model is selected, the theorist defines the emergent property, the measurable  
 122 signal of scientific interest. To continue our running STG example, one such emergent property  
 123 is the phenomenon of *network syncing* – in certain parameter regimes, the frequency of the hub  
 124 neuron matches that of the fast and slow populations at an intermediate frequency. This emergent  
 125 property is shown in Figure 1A at a frequency of 0.55Hz.

126 Third, qualitative parameter analysis ensues: since precise mathematical analysis is intractable in  
 127 this model, a brute force sweep of parameters is done [20]. Subsequently, a qualitative description is  
 128 formulated to describe of 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: the black box in Figure 1A takes, as input, the model and the specified  
 134 emergent property, and produces as output the parameter distribution shown in Figure 1B. This  
 135 distribution – represented for clarity as samples from the distribution – is then a scientifically  
 136 meaningful and mathematically tractable object. It conveys parameter regions critical to the emer-  
 137 gent property, directions in parameter space that will be invariant (or not) to that property, and  
 138 more. In the STG model, this distribution can be specifically queried to determine the prototypical  
 139 parameter configuration for network syncing (the mode; Figure 1B star), and then how quickly  
 140 network syncing will decay based on changes away from that mode. The inset of Figure 1B vali-  
 141 dates that indeed network syncing behaves as the distribution predicts, when moving away from  
 142 the mode (Figure 1B star). Further validation of EPI is available in the supplementary materials,  
 143 where we analyze a simpler model for which ground-truth statements can be made (Section A.1.1).

### 144 3.2 A deep generative modeling approach to emergent property inference

145 Emergent property inference (EPI) systematizes the three-step procedure of the previous section.  
 146 First, we consider the model as a coupled set of differential (and potentially stochastic) equations  
 147 [20]. In the running STG example, the dynamical state  $x = [x_{f1}, x_{f2}, x_{hub}, x_{s1}, x_{s2}]$  is the membrane  
 148 potential for each neuron, which evolves according to the biophysical conductance-based equation:

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

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

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

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

which completes the quantification of the emergent property.

Third, we perform emergent property inference: we find a distribution over parameter configurations  $z$ , and insist that samples from this distribution produce the emergent property; in other words, they obey the constraints introduced in Equation 2. This distribution will be chosen from a family of probability distributions  $\mathcal{Q} = \{q_\theta(z) : \theta \in \Theta\}$ , defined by a deep generative distribution of the normalizing flow class [15, 16, 17] – neural networks which transform a simple distribution into a suitably complicated distribution (as is needed here). This deep distribution is represented in Figure 1C (and see Methods for more detail). Then, mathematically, we must solve the following optimization program:

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

where  $T(x), \mu$  are defined as in Equation 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 [28, 29, 18, 30], but we emphasize that

<sup>174</sup> the EPI method is unaffected by this choice (but the results of course will depend on the primal  
<sup>175</sup> objective chosen).

<sup>176</sup> EPI optimizes the weights and biases  $\theta$  of the deep neural network (which induces the probability  
<sup>177</sup> distribution) by iteratively solving Equation 3. The optimization is complete when the sampled  
<sup>178</sup> models with parameters  $z \sim q_\theta$  produce activity consistent with the specified emergent property.  
<sup>179</sup> Such convergence is evaluated with a hypothesis test that the mean of each emergent property  
<sup>180</sup> statistic is not different than its emergent property value (see Section A.1.2). Equipped with this  
<sup>181</sup> method, we now prove out the value of EPI by using it to investigate three prominent models in  
<sup>182</sup> neuroscience, using EPI to produce new insights about these models.

<sup>183</sup> **3.3 Comprehensive input-responsivity in a nonlinear sensory system**

<sup>184</sup> In studies of primary visual cortex (V1), theoretical models with excitatory (E) and inhibitory  
<sup>185</sup> (I) populations have reproduced a host of experimentally documented phenomena. In particular  
<sup>186</sup> regimes of excitation and inhibition, these E/I models exhibit the paradoxical effect [4], selective  
<sup>187</sup> amplification [31], surround suppression [32], and sensory integrative properties [33]. Extending  
<sup>188</sup> this model using experimental evidence of three genetically-defined classes of inhibitory neurons  
<sup>189</sup> [34, 35], recent work [21] has investigated a four-population model – excitatory (E), parvalbumin  
<sup>190</sup> (P), somatostatin (S), and vasointestinal peptide (V) neurons – as shown in Fig. 2A. The dynamical  
<sup>191</sup> state of this model is the firing rate of each neuron-type population  $x = [x_E, x_P, x_S, x_V]^\top$ , which  
<sup>192</sup> evolves according to rectified ( $\llbracket \cdot \rrbracket_+$ ) and exponentiated dynamics:

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

<sup>193</sup> with effective connectivity weights  $W$  and input  $h$ . In our analysis, we set the time constant  
<sup>194</sup>  $\tau = 20\text{ms}$  and dynamics coefficient  $n = 2$ . Also, as is fairly standard, we obtain an informative  
<sup>195</sup> estimate of the effective connectivities between these neuron-types  $W$  in mice by multiplying their  
<sup>196</sup> probability of connection with their average synaptic strength [36, 37] (see Section A.2.2). Given  
<sup>197</sup> these fixed choices of  $W$ ,  $n$ , and  $\tau$ , we studied the system’s response to input

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

<sup>198</sup> where the input  $h$  is comprised of a baseline input  $b = [b_E, b_P, b_S, b_V]^\top$  and a differential input  
<sup>199</sup>  $dh = [dh_E, dh_P, dh_S, dh_V]^\top$  to each neuron-type population. Throughout subsequent analyses, the  
<sup>200</sup> baseline input is  $b = [1, 1, 1, 1]^\top$ .

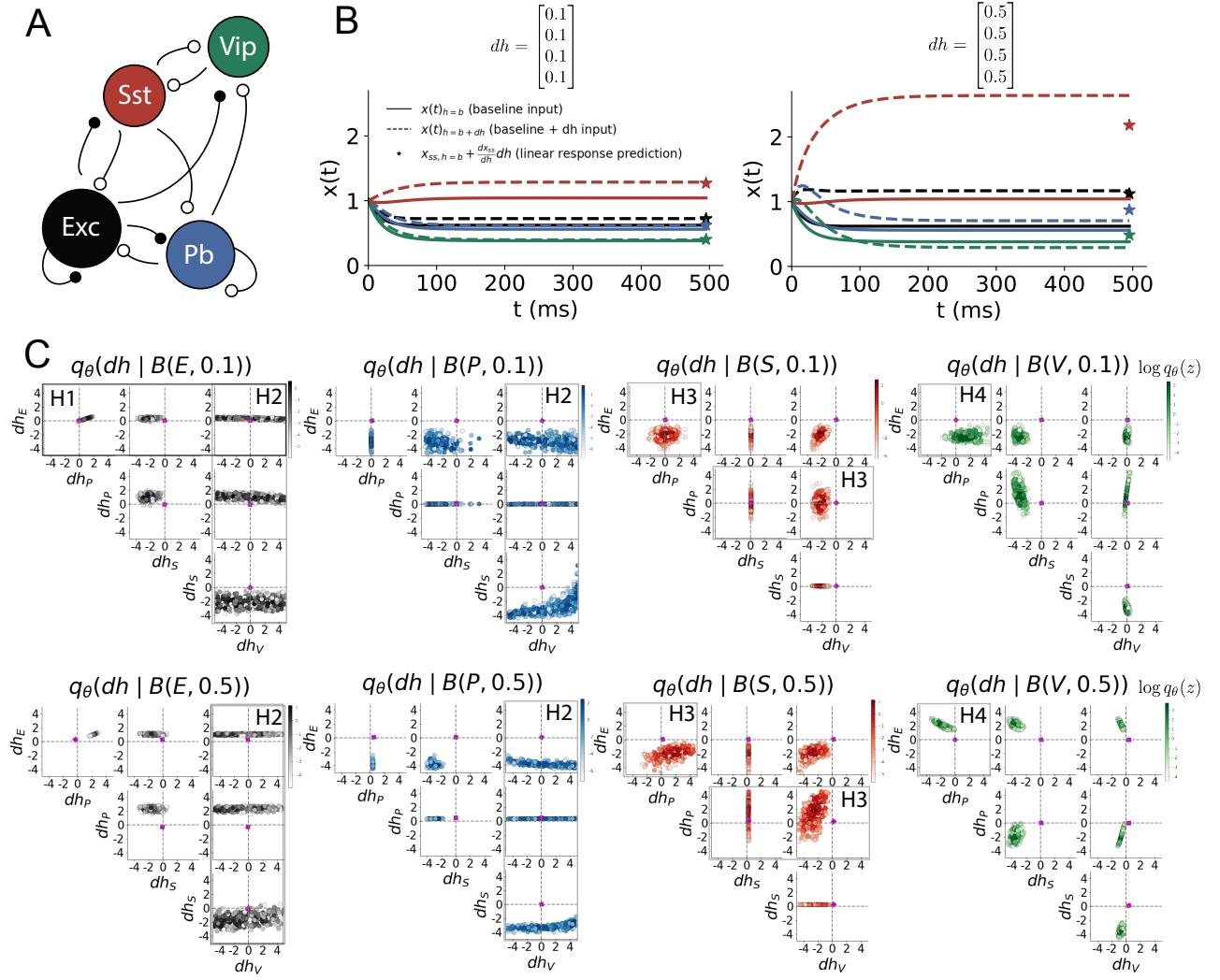


Figure 2: Hypothesis generation through EPI in a V1 model. A. Four-population model of primary visual cortex with excitatory (black), parvalbumin (blue), somatostatin (red), and vip (green) neurons. Some neuron-types largely do not form synaptic projections to others (excitatory and inhibitory projections filled and unfilled, respectively). B. Linear response predictions become inaccurate with greater input strength. V1 model simulations for input ( $b$ ) solid and ( $b + dh$ ) dashed.  $b = [1, 1, 1, 1]^T$  and (left)  $dh = [0.1, 0.1, 0.1, 0.1]^T$  (right)  $dh = [0.5, 0.5, 0.5, 0.5]^T$ . Stars indicate the linear response prediction. C. EPI distributions on differential input  $dh$  conditioned on differential response  $B(\alpha, y)$ . 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).

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

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

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

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

221

- 222 H1: as is intuitive, each neuron-type's firing rate should be sensitive to that neuron-type's direct input (e.g. Fig. 2C H1 indicates low variance in  $dh_E$  when  $\alpha = E$ . Same observation in all inferred distributions);
- 225 H2: the E- and P-populations should be largely unaffected by  $dh_V$  (Fig. 2C H2 indicates high variance in  $dh_V$  when  $\alpha \in \{E, P\}$ );
- 227 H3: the S-population should be largely unaffected by  $dh_P$  (Fig. 2C H3 indicate high variance in  $dh_P$  when  $\alpha = S$ );
- 229 H4: there should be a nonmonotonic response of  $dx_{V,ss}$  with  $dh_E$  (Fig. 2C H4 indicates that negative  $dh_E$  should result in small  $dx_{V,ss}$ , but positive  $dh_E$  should elicit a larger  $dx_{V,ss}$ );

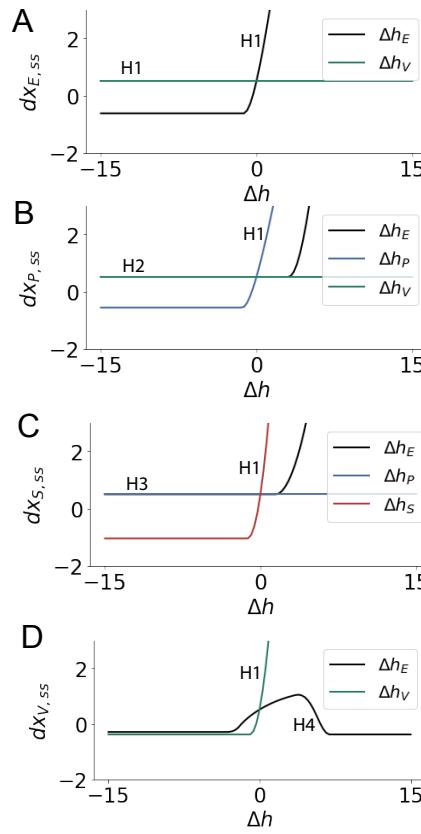


Figure 3: Confirming EPI generated hypotheses in V1. A. Differential responses by the E-population to changes in individual input  $\Delta h_\alpha u_\alpha$  away from the mode of the EPI distribution  $dh^*$ . B-D Same plots for the P-, S-, and V-populations. Labels H1, H2, H3, and H4 indicate which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

231 We evaluate these hypotheses by taking steps in individual neuron-type input  $\Delta h_\alpha$  away from the  
232 modes of the inferred distributions at  $y = 0.1$ .

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

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

- 235 • the neuron-type responses are sensitive to their direct inputs (Fig. 3A black, 3B blue, 3C  
236 red, 3D green);
- 237 • the E- and P-populations are not affected by  $dh_V$  (Fig. 3A green, 3B green);
- 238 • the S-population is not affected by  $dh_P$  (Fig. 3C blue);
- 239 • the V-population exhibits a nonmonotonic response to  $dh_E$  (Fig. 3D black), and is in fact  
240 the only population to do so (Fig. 3A-C black).

241 These hypotheses were in stark contrast to what was available to us via traditional analytical linear  
242 prediction (Fig. 2C, magenta). To this point, we have shown the utility of EPI on relatively low-  
243 level emergent properties like network syncing and differential neuron-type population responses.

<sup>244</sup> In the remainder of the study, we focus on using EPI to understand models of more abstract  
<sup>245</sup> cognitive function.

<sup>246</sup> **3.4 Identifying neural mechanisms of behavioral learning.**

<sup>247</sup> Identifying measurable biological changes that result in improved behavior is important for neuro-  
<sup>248</sup> science, since they may indicate how the learning brain adapts. In a rapid task switching exper-  
<sup>249</sup> iment [38], where rats were to respond right (R) or left (L) to the side of a light stimulus in the  
<sup>250</sup> pro (P) task, and oppositely in the anti (A) task predicated by an auditory cue (Fig. 3A), neural  
<sup>251</sup> recordings exhibited two population of neurons in each hemisphere of superior colliculus (SC) that  
<sup>252</sup> simultaneously represented both task condition and motor response: the Pro/contralateral and  
<sup>253</sup> Anti/ipsilateral neurons [22]. Duan et al. proposed a model of SC that, like the V1 model analyzed  
<sup>254</sup> in the previous section, is a four-population dynamical system. Here, the neuron-type populations  
<sup>255</sup> are functionally-defined as the Pro- and Anti-populations in each hemisphere (left (L) and right  
<sup>256</sup> (R)). The Pro- or Anti-populations receive an input determined by the cue, and then the left and  
<sup>257</sup> right populations receive an input based on the side of the light stimulus. Activities were bounded  
<sup>258</sup> between 0 and 1, so that a high output of the Pro population in a given hemisphere corresponds  
<sup>259</sup> to the contralateral response. An additional stipulation is that when one Pro population responds  
<sup>260</sup> with a high-output, the opposite Pro population must respond with a low output. Finally, this  
<sup>261</sup> circuit operates in the presence of gaussian noise resulting in trial-to-trial variability (see Section  
<sup>262</sup> A.2.3). The connectivity matrix is parameterized by the geometry of the population arrangement  
<sup>263</sup> (Fig. 3B).

<sup>264</sup> Here, we used EPI to learn distributions of the SC weight matrix parameters  $z = W$  conditioned  
<sup>265</sup> on of various levels of rapid task switching accuracy  $\mathcal{B}(p)$  for  $p \in \{50\%, 60\%, 70\%, 80\%, 90\%\}$  (see  
<sup>266</sup> Section A.2.3). As is standard, we decomposed the connectivity matrix  $W = QAQ^{-1}$  in such a  
<sup>267</sup> way (the Schur decomposition) that the basis vectors  $q_i$  are the same for all  $W$  (Fig. 3C). These  
<sup>268</sup> basis vectors have intuitive roles in processing for this task, and are accordingly named the *all*  
<sup>269</sup> mode - all neurons co-fluctuate, *side* mode - one side dominates the other, *task* mode - the Pro  
<sup>270</sup> or Anti populations dominate the other, and *diag* mode - Pro- and Anti-populations of opposite  
<sup>271</sup> hemispheres dominate the opposite pair. The corresponding eigenvalues (e.g.  $a_{\text{task}}$ , which change  
<sup>272</sup> according to  $W$ ) indicate the degree to which activity along that mode is increased or decreased  
<sup>273</sup> by  $W$ .

<sup>274</sup> EPI demonstrates that, for greater task accuracies, the task mode eigenvalue increases, indicating

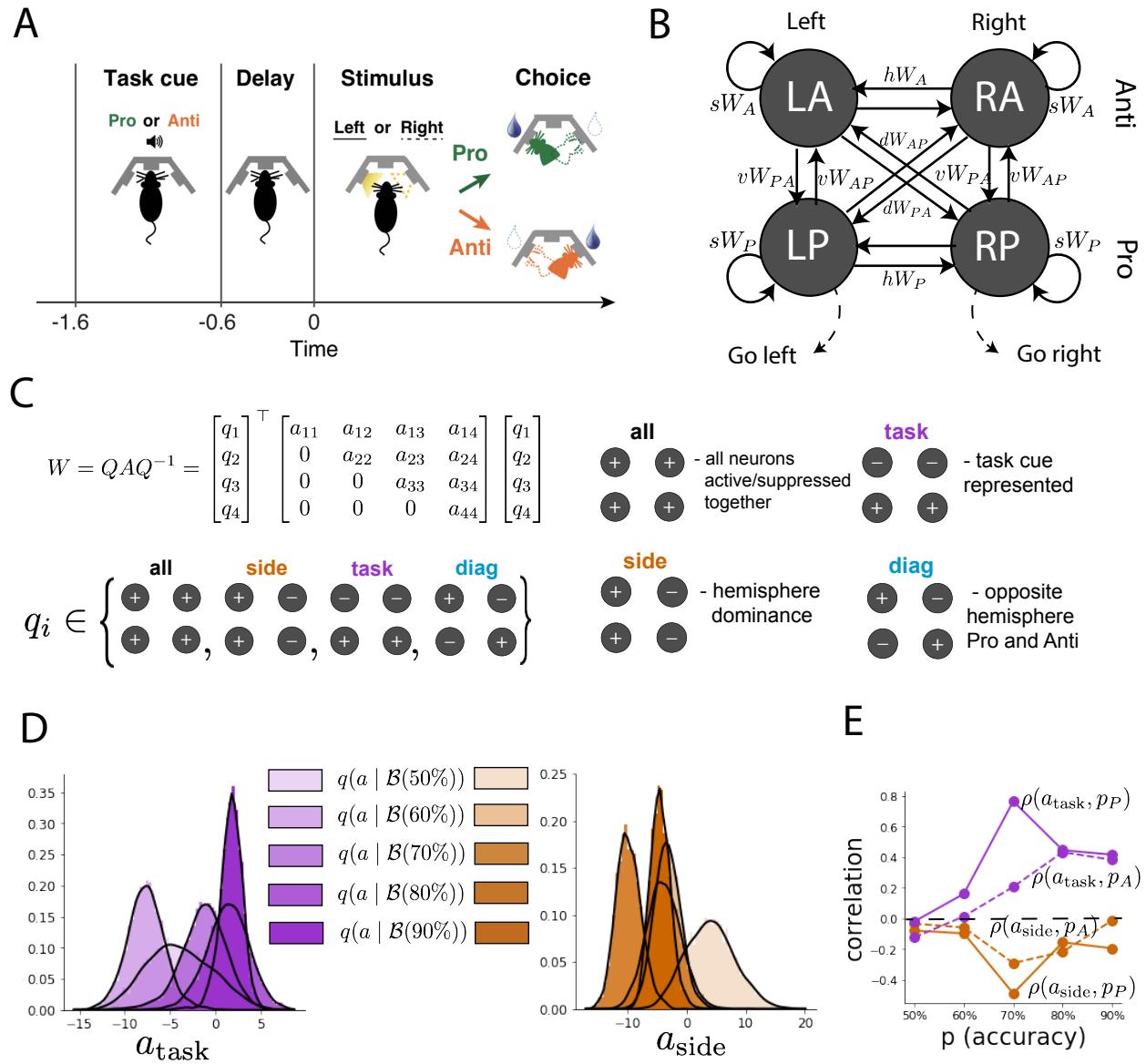


Figure 4: EPI reveals changes in SC [22] connectivity that result in greater task accuracy. A. Rapid task switching behavioral paradigm. In the Pro (Anti) condition indicated by an auditory cue, rats respond by poking into a side port to the same (opposite) side as the light stimulus that is provided after a delay to receive a reward. B. Model of superior colliculus (SC). Neurons: LP - left pro, RP - right pro, LA - left anti, RA - right anti. Parameters:  $sW$  - self,  $hW$  - horizontal,  $vW$  - vertical,  $dW$  - diagonal weights. C. The Schur decomposition of the weight matrix  $W = QAQ^{-1}$  is a unique decomposition with orthogonal  $Q$  and upper triangular  $A$ . The invariant Schur modes are labeled by their hypothesized role in computation:  $q_{all}$ ,  $q_{task}$ ,  $q_{side}$ , and  $q_{diag}$ . The values of  $A$  are what change for different realizations of  $W$ . 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.

the importance of  $W$  to the task representation (Fig. 4D, purple). Stepping from random chance (50%) networks to marginally task-performing (60%) networks, there is a marked decrease of the side mode eigenvalues (Fig. 3D, orange). Such side mode suppression remains in the models achieving greater accuracy, revealing its importance towards task performance. There were no interesting trends with learning in the all or diag mode (hence not shown in Fig. 3). 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. 3E). Thus, EPI produces novel, experimentally testable predictions: effective connectivity between these populations changes throughout learning, in a way that increases its task mode and decreases its side mode eigenvalues.

### 3.5 Characterizing the sources of bias in RNN computation

Each model we thus far 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 models of computation and have become increasingly popular in neuroscience research [39]. Typically, 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. Here we run EPI on the connectivity matrices of RNNs trained to solve a sample task.

Recent work establishes a link between RNN connectivity weights and the resulting dynamical responses of the network, using dynamic mean field theory (DMFT) [3]. Specifically, DMFT describes the properties of activity in infinite-size neural networks given a distribution on the connectivity weights. This theory has been extended from random neural networks to low-rank RNNs, which have low-dimensional parameterizations of RNN connectivity via the pairwise correlations of the low-rank vectors (i.e. the low-rank “geometry”) [23]. In such a model, the connectivity of a rank-1 RNN’s weight matrix  $J$  is the sum of a random component with strength determined by  $g$  and a structured component determined by the outer product of vectors  $m$  and  $n$ :

$$J = g\chi + \frac{1}{N}mn^\top, \quad (8)$$

where the activity  $x$  evolves as

$$\frac{dx}{dt} = -x(t) + J\phi(x(t)) + I(t), \quad (9)$$

and  $I(t)$  is some input,  $\phi$  is the tanh nonlinearity, and  $\chi_{ij} \sim \mathcal{N}(0, \frac{1}{N})$ . The entries of  $m$  and  $n$  are drawn from gaussian distributions  $m_i \sim \mathcal{N}(M_m, 1)$  and  $n_i \sim \mathcal{N}(M_n, 1)$ .

Mastrogiovanni et al. designed low-rank connectivities via the pairwise correlations of the vectors  $m, n$  in models that solve tasks from behavioral neuroscience. We can consider the DMFT equation solver as a black box that takes in a low-rank parameterization  $z$  (e.g.  $z = [g, M_m, M_n]$ ) and outputs task-relevant response variables (e.g. average network activity  $\mu$ , the temporal variability in the network  $\Delta_T$ , or network activity along a given dimension  $\kappa$ ). Importantly, the solution produced by the solver is differentiable with respect to the input parameters, allowing us to combine DMFT with EPI to learn distributions on such connectivity parameters of RNNs that execute tasks via an emergent property defined on the task-relevant responses produced by DMFT.

We train the network to solve gaussian posterior conditioning: calculate the parameters of a gaussian posterior distribution on the mean of a gaussian likelihood  $\mu_y$ , given a single observation of  $y \sim \mathcal{N}(\mu_y, 1)$  and a prior  $p(\mu_y) = \mathcal{N}(4, 1)$  (Fig. 5A). The true posterior for an input of  $y = 2$  is  $p(\mu_y | y) = \mathcal{N}(3, 0.5)$ . We used EPI to learn distributions of RNNs producing the correct posterior mean and variance in their mean activity  $\mu = \mu_{\text{post}}$  and temporal variance  $\Delta_T = \sigma_{\text{post}}^2$  (respectively), given an input of  $y = 2$ . (see Section A.2.4) (Fig. 5B).

When specifying the emergent property of gaussian posterior conditioning, we allowed a substantial amount of variability in the second moment constraints of the network mean  $\mu$  and temporal variance  $\Delta_T$ . This resulted in a distribution of rank-1 RNN parameterizations having a wide variety of biases in the resulting  $\mu_{\text{post}}$  and  $\sigma_{\text{post}}^2$  (under- or over-estimates of the posterior means and variances). We can examine the nature of the biases in this computation by visualizing the produced posterior means (Fig. 5B, left) and variances (Fig. 5B, right) in the EPI distribution. The inferred distribution has rough symmetry in the  $M_m$ - $M_n$  plane, suggesting a degeneracy in the product of  $M_m$  and  $M_n$  (Fig. 5B). The product of  $M_m$  and  $M_n$  almost completely determines the posterior mean (Fig. 5B, left), and the random strength  $g$  is the most influential variable on the temporal variance (Fig. 5B, right). Neither of these observations were obvious from the consistency equations afforded by DMFT (see Section A.2.4).

When working with DMFT, it's important to check that finite-size realizations of these infinite-size networks match the theoretical predictions. We check 2,000-neuron realizations of drawn parameters  $z_1$  and  $z_2$  from the inferred distribution.  $z_1$  has relatively high  $g$  and high  $M_m M_n$ , whereas  $z_2$  has relatively low  $g$  and low  $M_m M_n$ . Confirming our intuition,  $z_1$  overestimates the posterior mean, since mean activity  $\mu(t) > 3$  (Fig. 5C, left cyan). In turn,  $z_2$  underestimates the

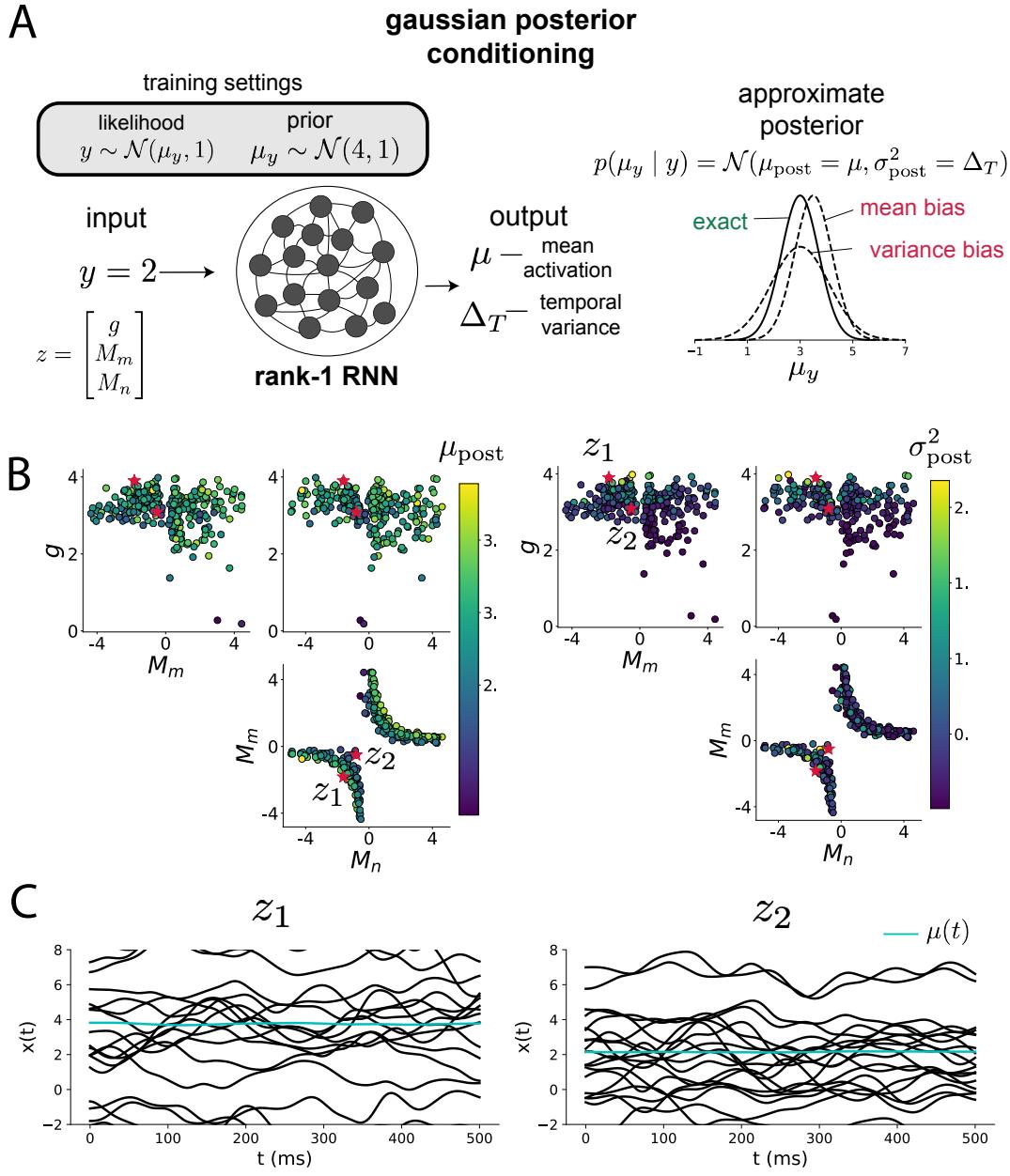


Figure 5: Sources of bias in RNN computation. A. (left) A rank-1 RNN running approximate Bayesian inference on  $\mu_y$  assuming a gaussian likelihood variance of 1 and a prior of  $\mathcal{N}(4, 1)$ . (center) The rank-1 RNN represents the computed gaussian posterior mean  $\mu_{\text{post}}$  and variance  $\sigma_{\text{post}}^2$  in its mean activity  $\mu$  and its temporal variance  $\Delta_T$ . (right) Bias in this computation can come from over- or under-estimating the posterior mean or variance. B. Distribution of rank-1 RNNs executing approximate Bayesian inference. Samples are colored by (left) posterior mean  $\mu_{\text{post}} = \mu$  and (right) posterior variance  $\sigma_{\text{post}}^2 = \Delta_T$ . C. Finite size realizations agree with the DMFT theory.

334 posterior mean, since  $\mu(t) < 3$  (Fig. 5C, right cyan). Finally,  $z_1$  results in evidently greater temporal  
 335 variance than  $z_2$ . This novel procedure of doing inference in interpretable parameterizations of  
 336 RNNs conditioned on task execution is straightforwardly generalizable to other tasks like noisy  
 337 integration and context-dependent decision making (Fig. S1).

## 338 4 Discussion

### 339 4.1 EPI is a general tool for theoretical neuroscience

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

350 In this study, we have focused on applying EPI to low dimensional parameter spaces of models  
 351 with low dimensional dynamical state. These choices were made to present the reader with a series  
 352 of interpretable conclusions, which is more challenging in high dimensional spaces. In fact, EPI  
 353 should scale reasonably to high dimensional parameter spaces, as the underlying technology has  
 354 produced state-of-the-art performance on high-dimensional tasks such as texture generation [18].  
 355 Of course, increasing the dimensionality of the dynamical state of the model makes optimization  
 356 more expensive, and there is a practical limit there as with any machine learning approach. For  
 357 systems with high dimensional state, we recommend using theoretical approaches (e.g. [23]) to  
 358 reason about reduced parameterizations of such high-dimensional systems.

359 There are additional technical considerations when assessing the suitability of EPI for a particu-  
 360 lar modeling question. First and foremost, as in any optimization problem, the defined emergent  
 361 property should always be appropriately conditioned (constraints should not have wildly different  
 362 units). Furthermore, if the program is underconstrained (not enough constraints), the distribution  
 363 grows (in entropy) unstably unless mapped to a finite support. If overconstrained, there is no pa-

364 parameter set producing the emergent property, and EPI optimization will fail (appropriately). Next,  
365 one should consider the computational cost of the gradient calculations. In the best circumstance,  
366 there is a simple, closed form expression (e.g. Section A.1.1) for the emergent property statistic  
367 given the model parameters. On the other end of the spectrum, many forward simulation iterations  
368 may be required before a high quality measurement of the emergent property statistic is available  
369 (e.g. Section A.2.1). In such cases, optimization will be expensive.

370 **4.2 Novel hypotheses from EPI**

371 Machine learning has played an effective, multifaceted role in neuroscientific progress. Primarily,  
372 it has revealed structure in large-scale neural datasets [40, 41, 42, 43, 44, 45] (see review, [14]).  
373 Secondarily, trained algorithms of varying degrees of biological relevance are beginning to be viewed  
374 as fully-observable computational systems comparable to the brain [46, 47].

375 For example, consider the fact that we do not fully understand the four-dimensional models of V1  
376 [21]. Because analytical approaches to studying nonlinear dynamical systems become increasingly  
377 complicated when stepping from two-dimensional to three- or four-dimensional systems in the  
378 absence of restrictive simplifying assumptions [48], it is unsurprising that this model has been a  
379 challenge. In Section 3.3, we showed that EPI was far more informative about neuron-type input  
380 responsivity than the predictions afforded through analysis. By flexibly conditioning this V1 model  
381 on different emergent properties, we performed an exploratory analysis of a *model* rather than a  
382 dataset, which generated and proved out a set of testable predictions.

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

389 In our final analysis, we present a novel procedure for doing statistical inference on interpretable  
390 parameterizations of RNNs executing simple tasks . This methodology relies on recently extended  
391 theory of responses in random neural networks with minimal structure [23]. With this methodology,  
392 we can finally open the probabilistic model selection toolkit reasoning about the connectivity of  
393 RNNs solving tasks.

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529 **A Methods**

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

531 Emergent property inference (EPI) learns distributions of theoretical model parameters that pro-  
 532 duce emergent properties of interest. EPI combines ideas from likelihood-free variational inference

[19] and maximum entropy flow networks [18]. A maximum entropy flow network is used as a deep probability distribution for the parameters, while these samples often parameterize a differentiable model simulator, which may lack a tractable likelihood function.

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

$$\mathcal{B} \leftrightarrow E_{z \sim q_\theta} [E_{x \sim p(x|z)} [T(x)]] = \mu \quad (10)$$

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

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

In most settings (especially those relevant to theoretical neuroscience) the likelihood of the behavior with respect to the model parameters  $p(T(x) | z)$  is unknown or intractable, requiring an alternative to stochastic gradient variational Bayes [5] or black box variational inference[49]. These types of methods called likelihood-free variational inference (LFVI, [19]) skate around the intractable likelihood function in situations where there is a differentiable simulator. Akin to LFVI, DSNs are optimized with the following objective for a given theoretical model, emergent property statistics  $T(x)$ , and emergent property constraints  $\mu$ :

$$\begin{aligned} q_\theta^*(z) &= \underset{q_\theta \in Q}{\operatorname{argmax}} H(q_\theta(z)) \\ \text{s.t. } E_{z \sim q_\theta} [E_{x \sim p(x|z)} [T(x)]] &= \mu \end{aligned} \quad (11)$$

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

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

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

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

561 that produce a band of oscillations. To do EPI with the dynamics matrix elements as the free  
 562 parameters  $z = [a_1, a_2, a_3, a_4]$ , and fixing  $\tau = 1$ , such that the posterior yields a band of oscillations,  
 563 the emergent property statistics  $T(x)$  are chosen to contain the first- and second-moments of the  
 564 oscillatory frequency  $\Omega$  and the growth/decay factor  $d$  of the oscillating system. To learn the  
 565 distribution of real entries of  $A$  that yield a distribution of  $d$  with mean zero with variance  $0.25^2$ ,  
 566 and oscillation frequency  $\Omega$  with mean 1 Hz with variance  $(0.1\text{Hz})^2$ , then we would select the real  
 567 part of the complex conjugate eigenvalues  $\text{real}(\lambda_1) = d$  (via an arbitrary choice of eigenvalue of the  
 568 dynamics matrix  $\lambda_1$ ) and the positive imaginary component of one of the eigenvalues  $\text{imag}(\lambda_1) =$   
 569  $2\pi\Omega$  as the emergent property statistics. Those emergent property statistics are then constrained  
 570 to

$$\mu = E \begin{bmatrix} \text{real}(\lambda_1) \\ \text{imag}(\lambda_1) \\ (\text{real}(\lambda_1) - 0)^2 \\ (\text{imag}(\lambda_1) - 2\pi\Omega)^2 \end{bmatrix} = \begin{bmatrix} 0.0 \\ 2\pi\Omega \\ 0.25^2 \\ (2\pi 0.1)^2 \end{bmatrix} \quad (12)$$

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

$$\lambda = \frac{\left(\frac{a_1+a_4}{\tau}\right) \pm \sqrt{\left(\frac{a_1+a_4}{\tau}\right)^2 + 4\left(\frac{a_2a_3-a_1a_4}{\tau}\right)}}{2} \quad (13)$$

574 where  $\lambda_1$  is the eigenvalue of  $\frac{1}{\tau}A$  with greatest real part. Even though  $E_{x \sim p(x|z)} [T(x)]$  is calculable  
 575 directly via a closed form function and does not require simulation, we cannot derive the distribution  
 576  $q_\theta^*$  directly. This is due to the formally hard problem of the backward mapping: finding the natural  
 577 parameters  $\eta$  from the mean parameters  $\mu$  of an exponential family distribution [50]. Instead, we  
 578 can use EPI to learn the linear system parameters producing such a band of oscillations (Fig. S2B).

579 Even this relatively simple system has nontrivial (though intuitively sensible) structure in the  
 580 parameter distribution. To validate our method (further than that of the underlying technology  
 581 on a ground truth solution [18]) we can analytically derive the contours of the probability density

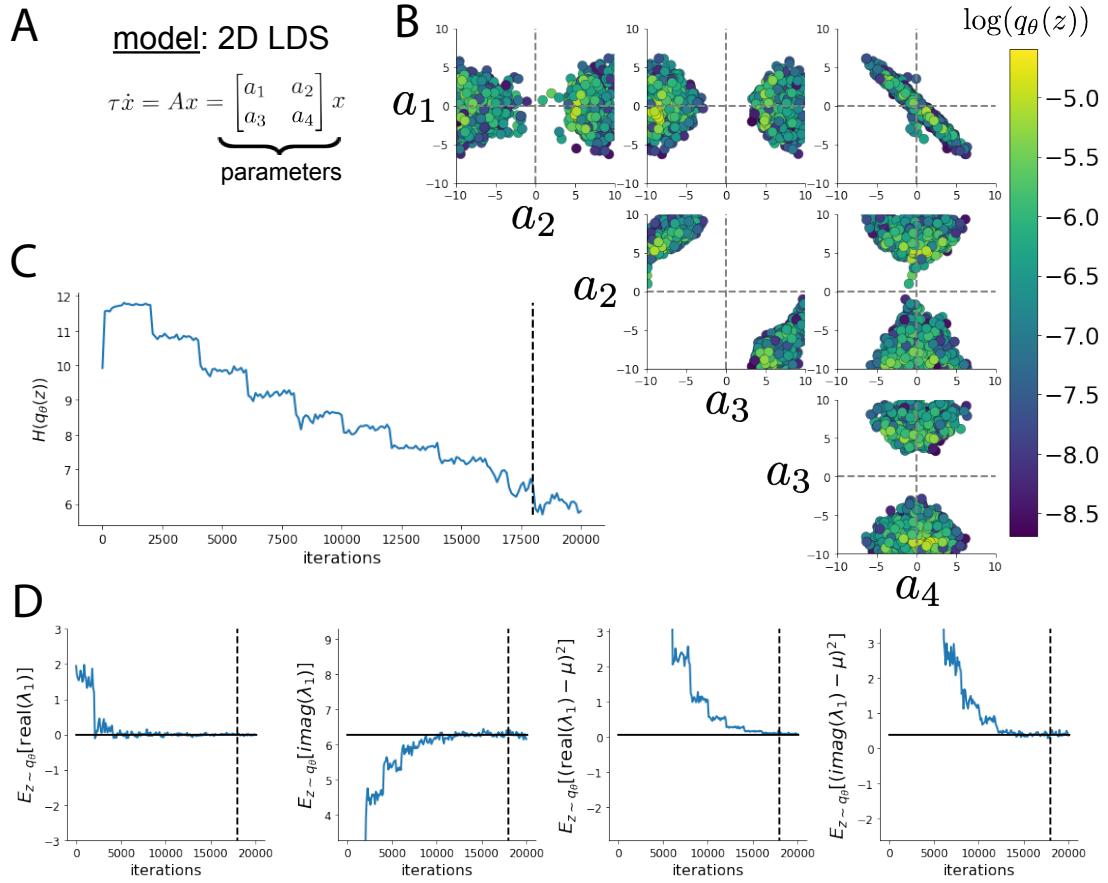


Fig. S2: A. Two-dimensional linear dynamical system model, where real entries of the dynamics matrix  $A$  are the parameters. B. The DSN distribution for a 2D LDS with  $\tau = 1$  that produces an average of 1Hz oscillations with some small amount of variance. C. Entropy throughout the optimization.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

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

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

$$\text{imag}(\lambda_1) = \begin{cases} \sqrt{\frac{a_1 a_4 - a_2 a_3}{\tau}}, & \text{if } a_1 a_4 < a_2 a_3 \\ 0 & \text{otherwise} \end{cases} \quad (14)$$

591 When  $\tau = 1$  and  $a_1 a_4 > a_2 a_3$  (center of distribution above), we have the following equation for the  
 592 other two dimensions:

$$\text{imag}(\lambda_1)^2 = a_1 a_4 - a_2 a_3 \quad (15)$$

593 Since we constrained  $E_{q_\theta}[\text{imag}(\lambda)] = 2\pi$  (with  $\omega = 1$ ), we can plot contours of the equation  
 594  $\text{imag}(\lambda_1)^2 = a_1 a_4 - a_2 a_3 = (2\pi)^2$  for various  $a_1 a_4$  (Fig. S3A). If  $\sigma_{1,4} = E_{q_\theta}(|a_1 a_4 - E_{q_\theta}[a_1 a_4]|)$ ,  
 595 then we plot the contours as  $a_1 a_4 = 0$  (black),  $a_1 a_4 = -\sigma_{1,4}$  (black dotted), and  $a_1 a_4 = -2\sigma_{1,4}$   
 596 (grey dotted) (Fig. S3B). This validates the curved structure of the inferred distribution learned  
 597 through EPI. We take steps in negative standard deviation of  $a_1 a_4$  (dotted and gray lines), since  
 598 there are few positive values  $a_1 a_4$  in the posterior. Subtler model-behavior combinations will have  
 599 even more complexity, further motivating the use of EPI for understanding these systems. Indeed,  
 600 we sample a distribution of systems oscillating near 1Hz (Fig. S4).

### 601 A.1.2 Augmented Lagrangian optimization

602 To optimize  $q_\theta(z)$  in equation 1, the constrained optimization is performed using the augmented  
 603 Lagrangian method. The following objective is minimized:

$$L(\theta; \alpha, c) = -H(q_\theta) + \alpha^\top \delta(\theta) + \frac{c}{2} \|\delta(\theta)\|^2 \quad (16)$$

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

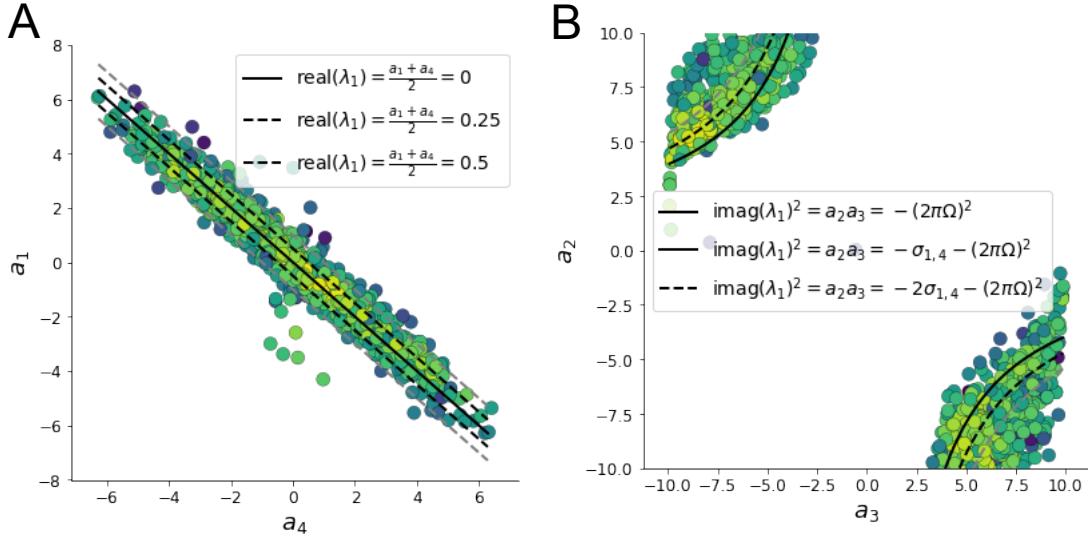


Fig. S3: A. Probability contours in the  $a_1 - a_4$  plane can be derived from the relationship to emergent property statistic of growth/decay factor. B. Probability contours in the  $a_2 - a_3$  plane can be derived from relationship to the emergent property statistic of oscillation frequency.

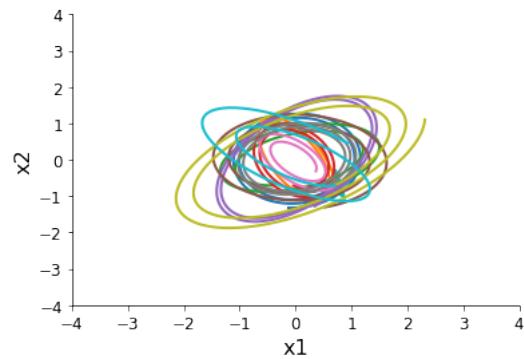


Fig. S4: Sampled dynamical system trajectories from the EPI distribution. Each trajectory is initialized at  $x(0) = \left[ \frac{\sqrt{2}}{2} \quad -\frac{\sqrt{2}}{2} \right]$ .

606 used initially, and increased during each augmented Lagrangian epoch – a period of optimization  
 607 with fixed  $\alpha$  and  $c$  for a given number of stochastic optimization iterations. Similarly,  $\alpha$  is tuned  
 608 each epoch based on the constraint violations. For the linear 2-dimensional system (Fig. S2C)  
 609 optimization hyperparameters are initialized to  $c_1 = 10^{-4}$  and  $\alpha_1 = 0$ . The penalty coefficient  
 610 is updated based on a hypothesis test regarding the reduction in constraint violation. The p-  
 611 value of  $E[|\delta(\theta_{k+1})|] > \gamma E[|\delta(\theta_k)|]$  is computed, and  $c_{k+1}$  is updated to  $\beta c_k$  with probability  
 612  $1 - p$ . Throughout the project,  $\beta = 4.0$  and  $\gamma = 0.25$  is used. The other update rule is  $\alpha_{k+1} =$   
 613  $\alpha_k + c_k \frac{1}{n} \sum_{i=1}^n (T(x^{(i)}) - \mu)$ . In this example, each augmented Lagrangian epoch ran for 2,000  
 614 iterations. We consider the optimization to have converged when a null hypothesis test of constraint  
 615 violations being zero is accepted for all constraints at a significance threshold 0.05. This is the dotted  
 616 line on the plots below depicting the optimization cutoff of EPI optimization for the 2-dimensional  
 617 linear system. If the optimization is left to continue running, entropy usually decreases, and  
 618 structural pathologies in the distribution may be introduced.

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

### 625 A.1.3 Normalizing flows

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

$$H(q_\theta(z)) = \int -q_\theta(z) \log(q_\theta(z)) dz = E_{z \sim q_\theta} [-\log(q_\theta(z))] = E_{\omega \sim q_0} [-\log(q_\theta(f_\theta(\omega)))] \quad (17)$$

$$\nabla_\theta H(q_\theta(z)) = E_{\omega \sim q_0} [-\nabla_\theta \log(q_\theta(f_\theta(\omega)))] \quad (18)$$

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

$$q(z') = q(f^{-1}(z')) \left| \det \frac{\partial f^{-1}(z')}{\partial z'} \right| = q(z) \left| \det \frac{\partial f(z)}{\partial z} \right|^{-1} \quad (19)$$

633 However, this computation has cubic complexity in dimensionality for fully connected layers. By  
 634 restricting our layers to normalizing flows [15] – bijective functions with fast log determinant ja-  
 635 cobian computations, we can tractably optimize deep generative models with objectives that are a  
 636 function of sample density, like entropy. Most of our analyses use real NVP [51], which have proven  
 637 effective in our architecture searches, and have the advantageous features of fast sampling and fast  
 638 density evaluation.

639 **A.1.4 Related work**

640 (To come)

641

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

643 (To come)

644

645 **A.2 Theoretical models**

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

648 **A.2.1 Stomatogastric ganglion**

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

$$C_m \frac{dx_m}{dt} = -[h_{leak}(x; z) + h_{Ca}(x; z) + h_K(x; z) + h_{hyp}(x; z) + h_{elec}(x; z) + h_{syn}(x; z)] \quad (20)$$

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

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

$$h_{leak}(x; z) = g_{leak}(x_m - V_{leak}) \quad (21)$$

$$h_{elec}(x; z) = g_{el}(x_m^{post} - x_m^{pre}) \quad (22)$$

$$h_{syn}(x; z) = g_{syn}S_\infty^{pre}(x_m^{post} - V_{syn}) \quad (23)$$

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

$$h_K(x; z) = g_KN(x_m - V_K) \quad (25)$$

$$h_{hyp}(x; z) = g_hH(x_m - V_{hyp}) \quad (26)$$

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

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

$$M_\infty = 0.5 \left( 1 + \tanh \left( \frac{x_m - v_1}{v_2} \right) \right) \quad (27)$$

$$\frac{dN}{dt} = \lambda_N(N_\infty - N) \quad (28)$$

$$N_\infty = 0.5 \left( 1 + \tanh \left( \frac{x_m - v_3}{v_4} \right) \right) \quad (29)$$

$$\lambda_N = \phi_N \cosh \left( \frac{x_m - v_3}{2v_4} \right) \quad (30)$$

$$\frac{dH}{dt} = \frac{(H_\infty - H)}{\tau_h} \quad (31)$$

$$H_\infty = \frac{1}{1 + \exp \left( \frac{x_m + v_5}{v_6} \right)} \quad (32)$$

$$\tau_h = 272 - \left( \frac{-1499}{1 + \exp \left( \frac{-x_m + v_7}{v_8} \right)} \right) \quad (33)$$

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

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

$$S_\infty = \frac{1}{1 + \exp\left(\frac{v_{th} - x_m}{v_0}\right)} \quad (34)$$

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

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

684 Our original approach to measuring frequency was to take the max of the fast Fourier transform  
685 (FFT) of the simulated time series. There are a few key considerations here. One is resolution  
686 in frequency space. Each FFT entry will correspond to a signal frequency of  $\frac{F_s k}{N}$ , where  $N$  is  
687 the number of samples used for the FFT,  $F_s = \frac{1}{dt}$ , and  $k \in [0, 1, \dots, N - 1]$ . Our resolution is  
688 improved by increasing  $N$  and decreasing  $dt$ . Increasing  $N = T - b$ , where  $b$  is some fixed number  
689 of buffer burn-in initialization samples, necessitates an increase in simulation time steps  $T$ , which  
690 directly increases computational cost. Increasing  $F_s$  (decreasing  $dt$ ) increases system approximation  
691 accuracy, but requires more time steps before a full cycle is observed. At the level of  $dt = 0.025$ ,  
692 thousands of temporal samples were required for resolution of .01Hz. These challenges in frequency  
693 resolution with the discrete Fourier transform motivated the use of an alternative basis of complex  
694 exponentials. Instead, we used a basis of complex exponentials with frequencies from 0.0-1.0 Hz at  
695 0.01Hz resolution,  $\Phi = [0.0, 0.01, \dots, 1.0]^\top$

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

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

$$u_i = \frac{|\mathcal{X}_i|^\alpha}{\sum_{k=1}^N |\mathcal{X}_i(k)|^\alpha} \quad (35)$$

705 The frequency is then calculated as  $\Omega_i = u_i^\top \Phi$  with  $\alpha = 100$ .

706 Network syncing, like all other emergent properties in this work, are defined by the emergent  
 707 property statistics and values. The emergent property statistics are the first- and second-moments  
 708 of the firing frequencies. The first moments are set to 0.55Hz, while the second moments are set to  
 709 0.025Hz<sup>2</sup>.

$$E \begin{bmatrix} \Omega_{f1} \\ \Omega_{f2} \\ \Omega_{hub} \\ \Omega_{s1} \\ \Omega_{s2} \\ (\Omega_{f1} - 0.55)^2 \\ (\Omega_{f2} - 0.55)^2 \\ (\Omega_{hub} - 0.55)^2 \\ (\Omega_{s1} - 0.55)^2 \\ (\Omega_{s2} - 0.55)^2 \end{bmatrix} = \begin{bmatrix} 0.55 \\ 0.55 \\ 0.55 \\ 0.55 \\ 0.55 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \\ 0.025^2 \end{bmatrix} \quad (36)$$

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

714 **A.2.2 Primary visual cortex**

715 The dynamics of each neural populations average rate  $x = \begin{bmatrix} x_E \\ x_P \\ x_S \\ x_V \end{bmatrix}$  are given by:

$$\tau \frac{dx}{dt} = -x + [Wx + h]_+^n \quad (37)$$

716 Some neuron-types largely lack synaptic projections to other neuron-types [52], and it is popular

<sup>717</sup> to only consider a subset of the effective connectivities [21].

$$W = \begin{bmatrix} W_{EE} & W_{EP} & W_{ES} & 0 \\ W_{PE} & W_{PP} & W_{PS} & 0 \\ W_{SE} & 0 & 0 & W_{SV} \\ W_{VE} & W_{VP} & W_{VS} & 0 \end{bmatrix} \quad (38)$$

<sup>718</sup> Estimates of the probability of connection and strength of connection from the Allen institute  
<sup>719</sup> result in an estimate of the effective connectivity [?]:

$$W = \begin{bmatrix} 0.0576 & 0.19728 & 0.13144 & 0 \\ 0.58855 & 0.30668 & 0.4285 & 0 \\ 0.15652 & 0 & 0 & 0.2 \\ 0.13755 & 0.0902 & 0.4004 & 0 \end{bmatrix} \quad (39)$$

<sup>720</sup> We look at how this four-dimensional nonlinear dynamical model of V1 responds to different inputs,  
<sup>721</sup> and compare the predictions of the linear response to the approximate posteriors obtained through  
<sup>722</sup> EPI. The input to the system is the sum of a baseline input  $b = [1 \ 1 \ 1 \ 1]^\top$  and a differential  
<sup>723</sup> input  $dh$ :

$$h = b + dh \quad (40)$$

<sup>724</sup> All simulations of this system had  $T = 100$  time points, a time step  $dt = 5\text{ms}$ , and time constant  
<sup>725</sup>  $\tau = 20\text{ms}$ . And the system was initialized to a random draw  $x(0)_i \sim \mathcal{N}(1, 0.01)$ .

<sup>726</sup> We can describe the dynamics of this system more generally by

$$\dot{x}_i = -x_i + f(u_i) \quad (41)$$

<sup>727</sup> where the input to each neuron is

$$u_i = \sum_j W_{ij}x_j + h_i \quad (42)$$

<sup>728</sup> Let  $F_{ij} = \gamma_i \delta(i, j)$ , where  $\gamma_i = f'(u_i)$ . Then, the linear response is

$$\frac{dx_{ss}}{dh} = F(W \frac{dx_{ss}}{dh} + I) \quad (43)$$

<sup>729</sup> which is calculable by

$$\frac{dx_{ss}}{dh} = (F^{-1} - W)^{-1} \quad (44)$$

<sup>730</sup> The emergent property we considered was the first and second moments of the change in rate  $dx$   
<sup>731</sup> between the baseline input  $h = b$  and  $h = b + dh$ . We use the following notation to indicate that

<sup>732</sup> the emergent property statistics were set to the following values:

$$\mathcal{B}(\alpha, y) \leftrightarrow E \begin{bmatrix} dx_{\alpha,ss} \\ (dx_{\alpha,ss} - y)^2 \end{bmatrix} = \begin{bmatrix} y \\ 0.01^2 \end{bmatrix} \quad (45)$$

<sup>733</sup> In the final analysis for this model, we sweep the input one neuron at a time away from the mode  
<sup>734</sup> of each inferred distributions  $dh^* = z^* = \text{argmax}_z \log q_\theta(z | \mathcal{B}(\alpha, 0.1))$ . The differential responses  
<sup>735</sup>  $dx_{\alpha,ss}$  are examined at perturbed inputs  $h = b + dh^* + \Delta h_\alpha u_\alpha$  where  $u_\alpha$  is a unit vector in the  
<sup>736</sup> dimension of  $\alpha$  and  $\Delta h_\alpha \in [-15, 15]$ .

<sup>737</sup> For each  $\mathcal{B}(\alpha, y)$  with  $\alpha \in \{E, P, S, V\}$  and  $y \in \{0.1, 0.5\}$ , we ran EPI with five different random  
<sup>738</sup> initial seeds using an architecture of four coupling layers, each with two hidden layers of 10 units.  
<sup>739</sup> We set  $c_0 = 10^5$ . The support of the learned distribution was restricted to  $z_i \in [-5, 5]$ .

<sup>740</sup> **A.2.3 Superior colliculus**

<sup>741</sup> There are four total units: two in each hemisphere corresponding to the Pro/contralateral and  
<sup>742</sup> Anti/ipsilateral populations. Each unit has an activity ( $x_i$ ) and internal variable ( $u_i$ ) related by

$$x_i(t) = \left( \frac{1}{2} \tanh \left( \frac{v_i(t) - \epsilon}{\zeta} \right) + \frac{1}{2} \right) \quad (46)$$

<sup>743</sup>  $\epsilon = 0.05$  and  $\zeta = 0.5$  control the position and shape of the nonlinearity, respectively.

<sup>744</sup> We can order the elements of  $x_i$  and  $v_i$  into vectors  $x$  and  $v$  with elements

$$x = \begin{bmatrix} x_{LP} \\ x_{LA} \\ x_{RP} \\ x_{RA} \end{bmatrix} \quad v = \begin{bmatrix} v_{LP} \\ v_{LA} \\ v_{RP} \\ v_{RA} \end{bmatrix} \quad (47)$$

<sup>745</sup> The internal variables follow dynamics:

$$\tau \frac{dv}{dt} = -v + Wx + h + \sigma dB \quad (48)$$

<sup>746</sup> with time constant  $\tau = 0.09s$  and gaussian noise  $\sigma dB$  controlled by the magnitude of  $\sigma = 1.0$ . The  
<sup>747</sup> weight matrix has 8 parameters  $sW_P$ ,  $sW_A$ ,  $vW_{PA}$ ,  $vW_{AP}$ ,  $hW_P$ ,  $hW_A$ ,  $dW_{PA}$ , and  $dW_{AP}$  (Fig.  
<sup>748</sup> 4B).

$$W = \begin{bmatrix} sW_P & vW_{PA} & hW_P & dW_{PA} \\ vW_{AP} & sW_A & dW_{AP} & hW_A \\ hW_P & dW_{PA} & sW_P & vW_{PA} \\ dW_{AP} & hW_A & vW_{AP} & sW_A \end{bmatrix} \quad (49)$$

<sup>749</sup> The system receives five inputs throughout each trial, which has a total length of 1.8s.

$$h = h_{\text{rule}} + h_{\text{choice-period}} + h_{\text{light}} \quad (50)$$

<sup>750</sup> There are rule-based inputs depending on the condition,

$$h_{P,\text{rule}}(t) = \begin{cases} I_{P,\text{rule}} \begin{bmatrix} 1 & 0 & 0 & 1 \end{bmatrix}^\top, & \text{if } t \leq 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (51)$$

<sup>751</sup>

$$h_{A,\text{rule}}(t) = \begin{cases} I_{A,\text{rule}} \begin{bmatrix} 0 & 1 & 1 & 0 \end{bmatrix}^\top, & \text{if } t \leq 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (52)$$

<sup>752</sup> a choice-period input,

$$h_{\text{choice}}(t) = \begin{cases} I_{\text{choice}} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^\top, & \text{if } t > 1.2s \\ 0, & \text{otherwise} \end{cases} \quad (53)$$

<sup>753</sup> and an input to the right or left-side depending on where the light stimulus is delivered.

$$h_{\text{light}}(t) = \begin{cases} I_{\text{light}} \begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}^\top, & \text{if } t > 1.2s \text{ and Left} \\ I_{\text{light}} \begin{bmatrix} 0 & 0 & 1 & 1 \end{bmatrix}^\top, & \text{if } t > 1.2s \text{ and Right} \\ 0, & t \leq 1.2s \end{cases} \quad (54)$$

<sup>754</sup> The input parameterization was fixed to  $I_{P,\text{rule}} = 10$ ,  $I_{A,\text{rule}} = 10$ ,  $I_{\text{choice}} = 2$ , and  $I_{\text{light}} = 1$

<sup>755</sup> To produce a Bernoulli rate of  $p_{LP}$  in the Left, Pro condition (we can generalize this to either cue,

<sup>756</sup> or stimulus condition), let  $\hat{p}_i$  be the empirical average steady state (ss) response (final  $x_{LP}$  at end

<sup>757</sup> of task) over M=500 gaussian noise draws for a given SC model parameterization  $z_i$ :

$$\hat{p}_i = E_{\sigma dB} [x_{LP,ss} | s = L, c = P, z_i] = \frac{1}{M} \sum_{j=1}^M x_{LP,ss}(s = L, c = P, z_i, \sigma dB_j) \quad (55)$$

<sup>758</sup> For the first constraint, the average over posterior samples (from  $q_\theta(z)$ ) to be  $p_{LP}$ :

$$E_{z_i \sim q_\phi} [E_{\sigma dB} [x_{LP,ss} | s = L, c = P, z_i]] = E_{z_i \sim q_\phi} [\hat{p}_i] = p_{LP} \quad (56)$$

<sup>759</sup> We can then ask that the variance of the steady state responses across gaussian draws, is the

<sup>760</sup> Bernoulli variance for the empirical rate  $\hat{p}_i$ .

$$E_{z \sim q_\phi} [\sigma_{err}^2] = 0 \quad (57)$$

761

$$\sigma_{err}^2 = \text{Var}_{\sigma dB} [x_{LP,ss} | s = L, c = P, z_i] - \hat{p}_i(1 - \hat{p}_i) \quad (58)$$

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

$$E_{z \sim q_\phi} [d_P] = 1 \quad (59)$$

764

$$E_{\sigma dB} [(x_{LP,ss} - x_{RP,ss})^2 | s = L, c = P, z_i] \quad (60)$$

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

774 Training DSNs to learn distributions of dynamical system parameterizations that produce Bernoulli  
 775 responses at a given rate (with small variance around that rate) was harder to do than expected.  
 776 There is a pathology in this optimization setup, where the learned distribution of weights is bimodal  
 777 attributing a fraction  $p$  of the samples to an expansive mode (which always sends  $x_{LP}$  to 1), and a  
 778 fraction  $1 - p$  to a decaying mode (which always sends  $x_{LP}$  to 0). This pathology was avoided using  
 779 an inequality constraint prohibiting parameter samples that resulted in low variance of responses  
 780 across noise.

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

$$\mathcal{B}(p) \leftrightarrow \begin{bmatrix} \hat{p}_P \\ \hat{p}_A \\ (\hat{p}_P - p)^2 \\ (\hat{p}_A - p)^2 \\ \sigma_{P,err}^2 \\ \sigma_{A,err}^2 \\ d_P \\ d_A \end{bmatrix} = \begin{bmatrix} p \\ p \\ 0.15^2 \\ 0.15^2 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \quad (61)$$

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

784 **A.2.4 Rank-1 RNN**

785 The network dynamics of neuron  $i$ 's rate  $x$  evolve according to:

$$\dot{x}_i(t) = -x_i(t) + \sum_{j=1}^N J_{ij}\phi(x_j(t)) + I_i \quad (62)$$

786 where the connectivity is comprised of a random and structured component:

$$J_{ij} = g\chi_{ij} + P_{ij} \quad (63)$$

787 The random bulk component has elements drawn from  $\chi_{ij} \sim \mathcal{N}(0, \frac{1}{N})$ , and the structured component  
 788 is a sum of  $r$  unit rank terms:

$$P_{ij} = \sum_{k=1}^r \frac{m_i^{(k)} n_j^{(k)}}{N} \quad (64)$$

789 Rank-1 vectors  $m$  and  $n$  have elements drawn

$$m_i \sim \mathcal{N}(M_m, \Sigma_m)$$

790

$$n_i \sim \mathcal{N}(M_n, \Sigma_n)$$

791 The current has the following statistics:

$$I = M_I + \frac{\Sigma_{mI}}{\Sigma_m} x_1 + \frac{\Sigma_{nI}}{\Sigma_n} x_2 + \Sigma_\perp h$$

792 where  $x_1$ ,  $x_2$ , and  $h$  are standard normal random variables following the rank-1 input-driven example  
 793 from [23].

794 We followed their prescription for deriving the consistency equations in the presence of chaos. The  
 795  $\ddot{\Delta}$  equation is broken into the equation for  $\Delta_0$  and  $\Delta_\infty$  by the autocorrelation dynamics assertions.

$$\ddot{\Delta}(\tau) = -\frac{\partial V}{\partial \Delta}$$

796

$$\ddot{\Delta} = \Delta - \{g^2 \langle [\phi_i(t)\phi_i(t+\tau)] \rangle + \Sigma_m^2 \kappa^2 + 2\Sigma_{mI} \kappa + \Sigma_I^2\}$$

797 We can write out the potential function by integrating the negated RHS.

$$V(\Delta, \Delta_0) = \int \mathcal{D}\Delta \frac{\partial V(\Delta, \Delta_0)}{\partial \Delta}$$

798

$$V(\Delta, \Delta_0) = -\frac{\Delta^2}{2} + g^2 \langle [\Phi_i(t)\Phi_i(t+\tau)] \rangle + (\Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2)\Delta + C$$

799 We assume that as time goes to infinity, the potential relaxes to a steady state.

$$\frac{\partial V(\Delta_\infty, \Delta_0)}{\partial \Delta} = -\Delta + \{g^2 \langle [\phi_i(t)\phi_i(t+\infty)] \rangle + \Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2\} = 0$$

800

$$\Delta_\infty = g^2 \langle [\phi_i(t)\phi_i(t+\infty)] \rangle + \Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2$$

801 This can be written more explicitly in terms of the gaussian integrals which are relatively (with  
802 respect to nongaussian distributions) cheap to evaluate.

$$\Delta_\infty = g^2 \int \mathcal{D}z \left[ \int \mathcal{D}x \phi(\mu + \sqrt{\Delta_0 - \Delta_\infty}x + \sqrt{\Delta_\infty}z) \right]^2 + \Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2$$

803 Also, we assume that the energy of the system is preserved throughout the entirety of its evolution.

$$V(\Delta_0, \Delta_0) = V(\Delta_\infty, \Delta_0)$$

804

$$-\frac{\Delta_0^2}{2} + g^2 \langle [\Phi_i(t)\Phi_i(t)] \rangle + (\Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2)\Delta_0 + C = -\frac{\Delta_\infty^2}{2} + g^2 \langle [\Phi_i(t)\Phi_i(t)] \rangle + (\Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2)\Delta_\infty + C$$

805 We can arrange the terms into a difference of squares in  $\Delta_0$  and  $\Delta_\infty$ .

$$\frac{\Delta_0^2 - \Delta_\infty^2}{2} = g^2 (\langle [\Phi_i(t)\Phi_i(t)] \rangle - \langle [\Phi_i(t)\Phi_i(t)] \rangle) + (\Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2)(\Delta_0 - \Delta_\infty)$$

806 Similarly, we write out the resulting equation explicitly in terms of the gaussian integrals present.

$$\begin{aligned} \frac{\Delta_0^2 - \Delta_\infty^2}{2} &= g^2 \left( \int \mathcal{D}z \Phi^2(\mu + \sqrt{\Delta_0}z) - \int \mathcal{D}z \int \mathcal{D}x \Phi(\mu + \sqrt{\Delta_0 - \Delta_\infty}x + \sqrt{\Delta_\infty}z) \right) \\ &\quad + (\Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2)(\Delta_0 - \Delta_\infty) \end{aligned}$$

807  
808 This results in a set of consistency equations for the dynamic mean field variables  $\mu$ ,  $\kappa$ ,  $\Delta_0$ , and  
809  $\Delta_\infty$ . In order to obtain the values of these variables for a given parameterization, we must solve  
810 the following system of equations.

$$\begin{aligned} \mu &= F(\mu, \kappa, \Delta_0, \Delta_\infty) = M_m \kappa + M_I \\ \kappa &= G(\mu, \kappa, \Delta_0, \Delta_\infty) = M_n \langle [\phi_i] \rangle + \Sigma_{nI} \langle [\phi'_i] \rangle \\ \frac{\Delta_0^2 - \Delta_\infty^2}{2} &= H(\mu, \kappa, \Delta_0, \Delta_\infty) = g^2 \left( \int \mathcal{D}z \Phi^2(\mu + \sqrt{\Delta_0}z) - \int \mathcal{D}z \int \mathcal{D}x \Phi(\mu + \sqrt{\Delta_0 - \Delta_\infty}x + \sqrt{\Delta_\infty}z) \right) \\ &\quad + (\Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2)(\Delta_0 - \Delta_\infty) \\ \Delta_\infty &= L(\mu, \kappa, \Delta_0, \Delta_\infty) = g^2 \int \mathcal{D}z \left[ \int \mathcal{D}x \phi(\mu + \sqrt{\Delta_0 - \Delta_\infty}x + \sqrt{\Delta_\infty}z) \right]^2 + \Sigma_m^2 \kappa^2 + 2\Sigma_{mI}\kappa + \Sigma_I^2 \end{aligned} \tag{65}$$

<sup>811</sup> We can solve these equations by simulating the following Langevin dynamical system.

$$\begin{aligned}
 x(t) &= \frac{\Delta_0(t)^2 - \Delta_\infty(t)^2}{2} \\
 \Delta_0(t) &= \sqrt{2x(t) + \Delta_\infty(t)^2} \\
 \dot{\mu}(t) &= -\mu(t) + F(\mu(t), \kappa(t), \Delta_0(t), \Delta_\infty(t)) \\
 \dot{\kappa}(t) &= -\kappa + G(\mu(t), \kappa(t), \Delta_0(t), \Delta_\infty(t)) \\
 \dot{x}(t) &= -x(t) + H(\mu(t), \kappa(t), \Delta_0(t), \Delta_\infty(t)) \\
 \dot{\Delta_\infty}(t) &= -\Delta_\infty(t) + L(\mu(t), \kappa(t), \Delta_0(t), \Delta_\infty(t))
 \end{aligned} \tag{66}$$

<sup>812</sup> Then, the temporal variance, which is necessary for the gaussian posterior conditioning example, is  
<sup>813</sup> simply calculated via

$$\Delta_T = \Delta_0 - \Delta_\infty \tag{67}$$

### <sup>814</sup> A.3 Supplementary Figures

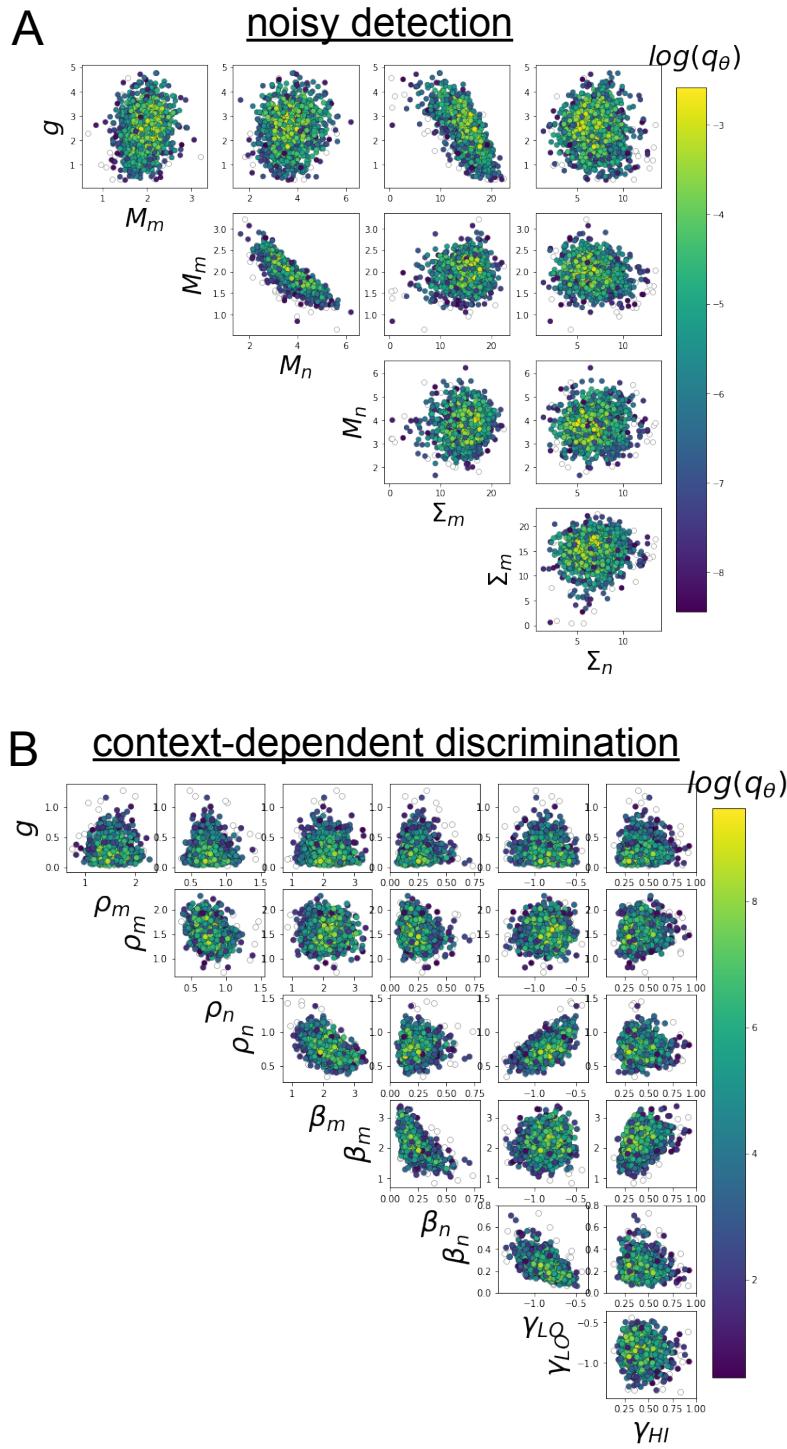


Fig. S1: A. EPI for rank-1 networks doing discrimination. B. EPI for rank-2 networks doing context-dependent discrimination.