Models of representation learning dynamics

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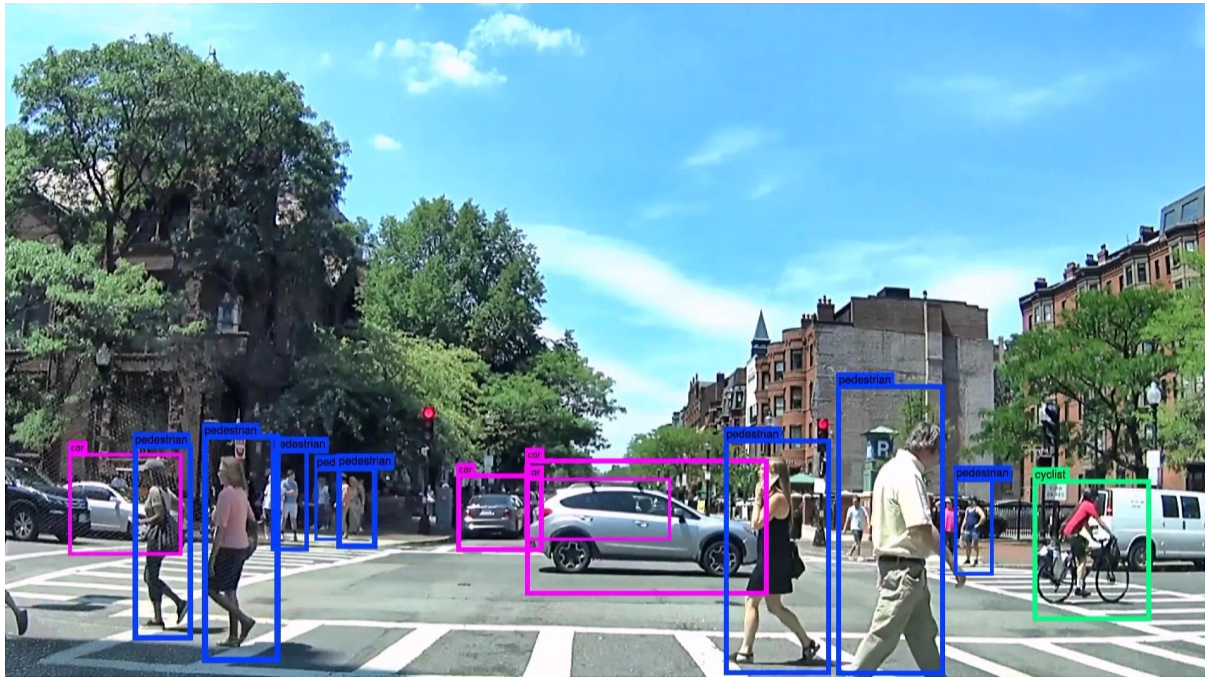
car
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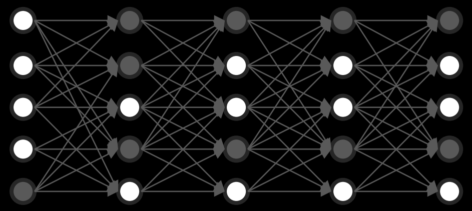
Artificial Intelligence



Neural Networks

Brain & Mind

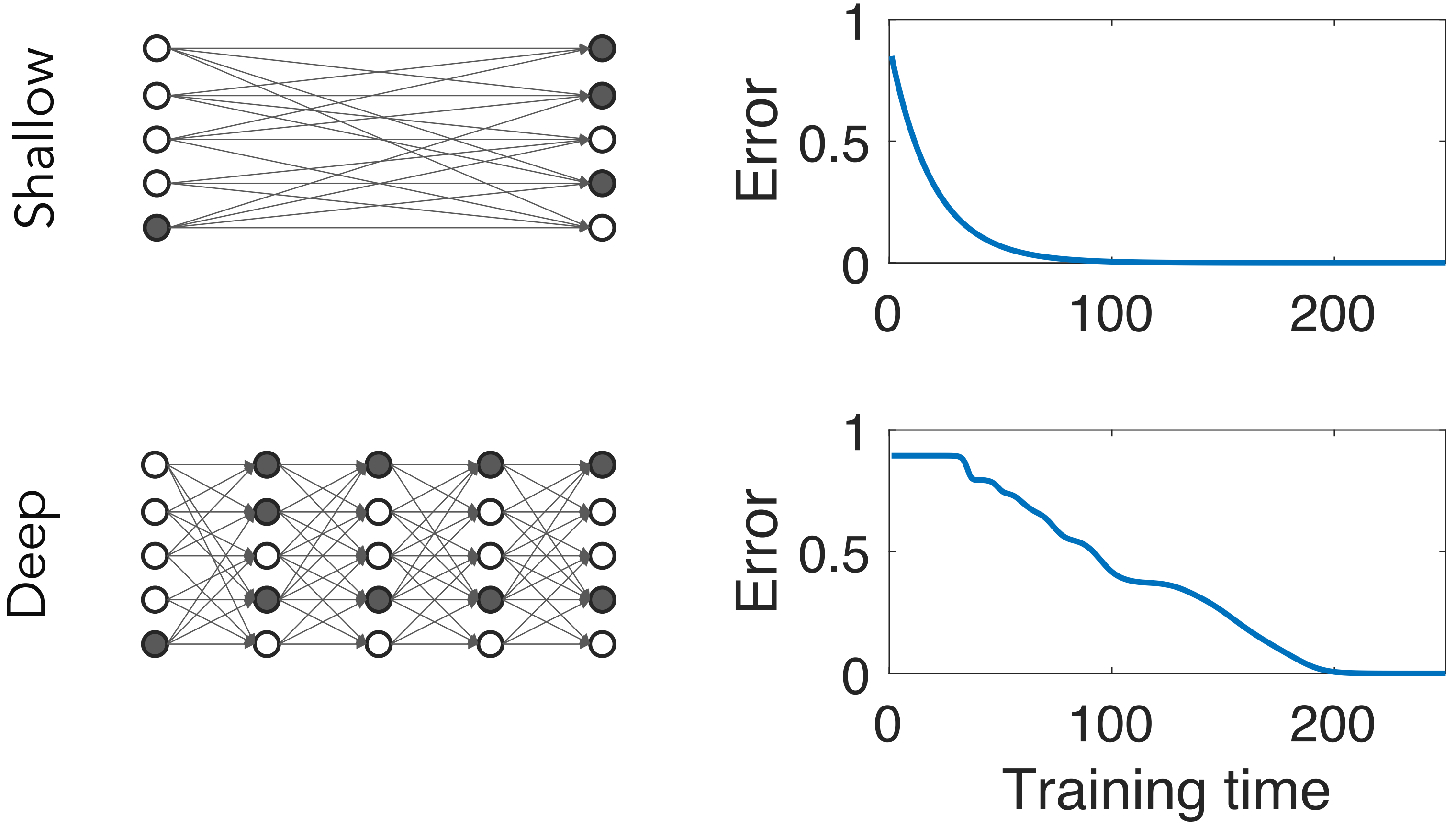
Today

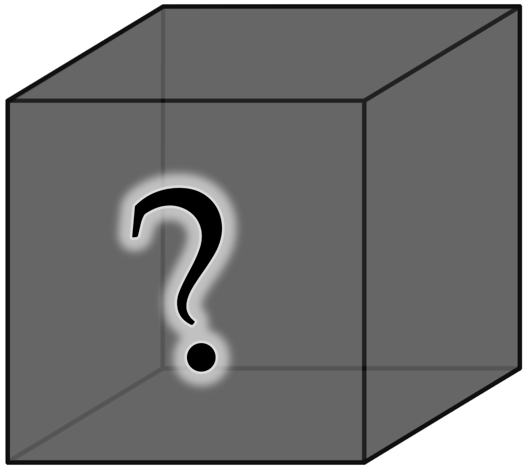
1. Deep linear network dynamics

2. Nontrivial initializations: Lazy, rich, & beyond

3. Nonlinear networks & the neural race reduction

Depth complicates learning dynamics





L. Zdeborová. Understanding deep learning is also a job for physicists. *Nature Physics*, 2020

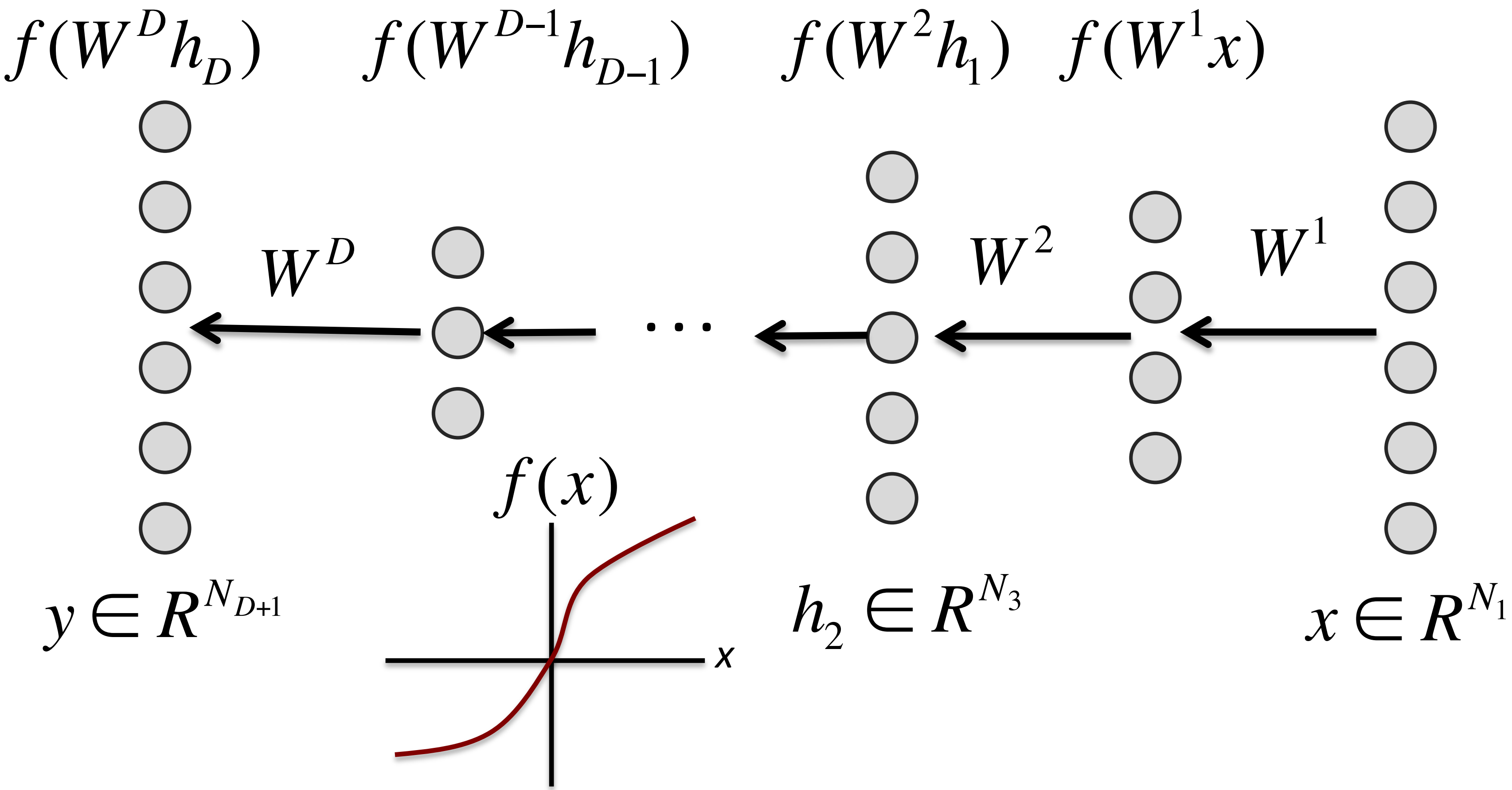
Credit: NYAS

Surrogate models

- Tackling these questions in full generality is challenging
- Instead, we can analyze a surrogate model that is simpler but retains key features of the full problem
- Particularly for brain sciences, crucial to have a minimal, tractable model
  - Conceptual clarity
  - Unambiguous predictions
  - Isolate contribution of depth, data statistics, nonlinearity

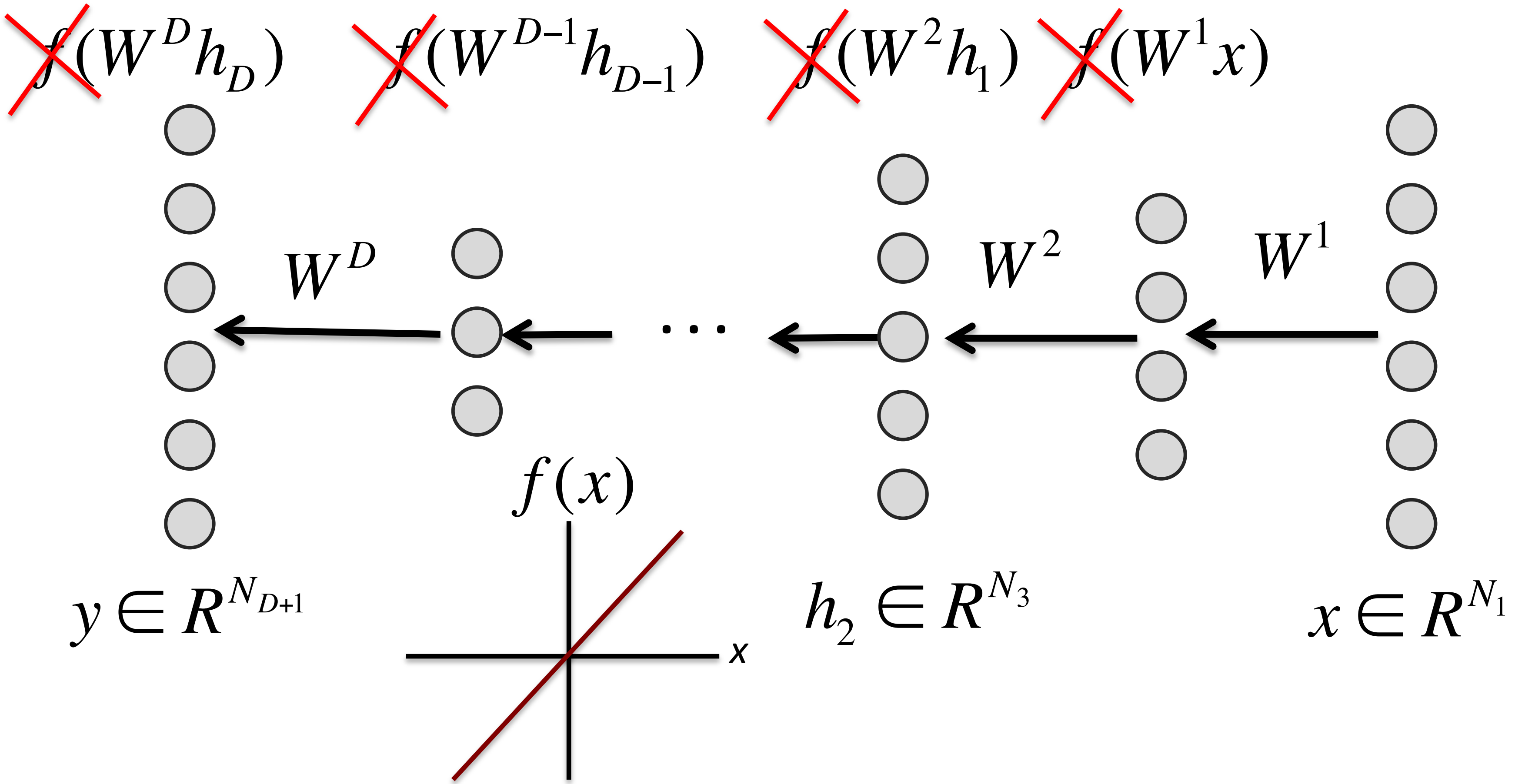
Deep network

- Little hope for a complete theory with arbitrary nonlinearities



Deep *linear* network

- Use a deep *linear* network as a starting point.



Gradient descent

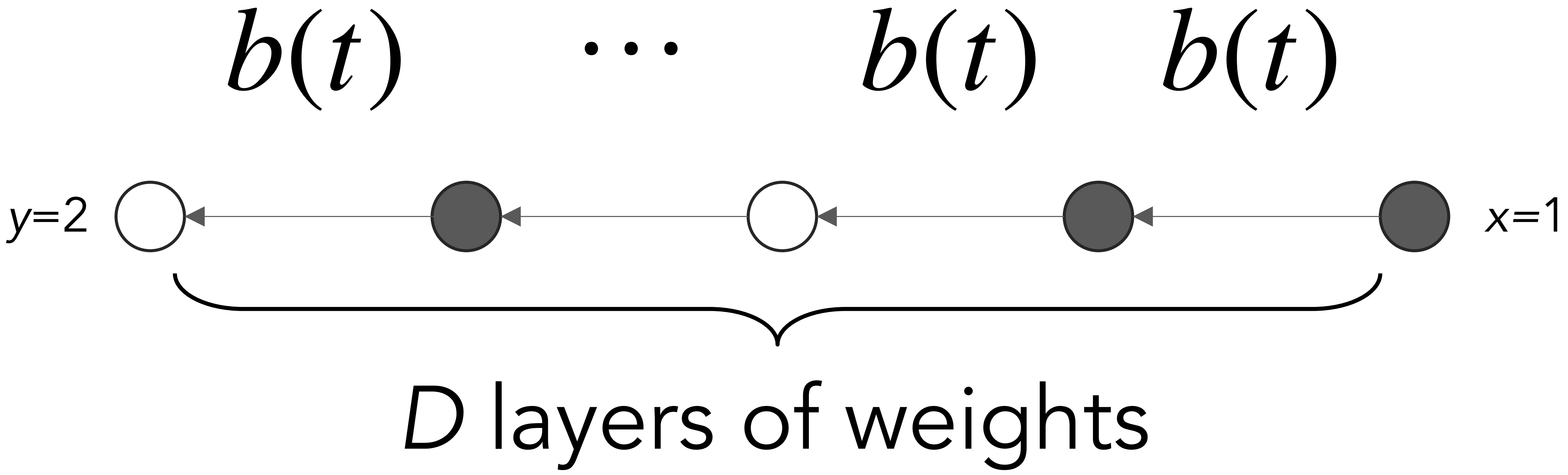
Mean squared error loss:

$$\min_{W_1,\cdots,W_D} \sum_{\mu} \left\| y^{\mu} - \left(\prod_{i=1}^{D} W^i \right) x^{\mu} \right\|^2$$

Gradient flow dynamics:

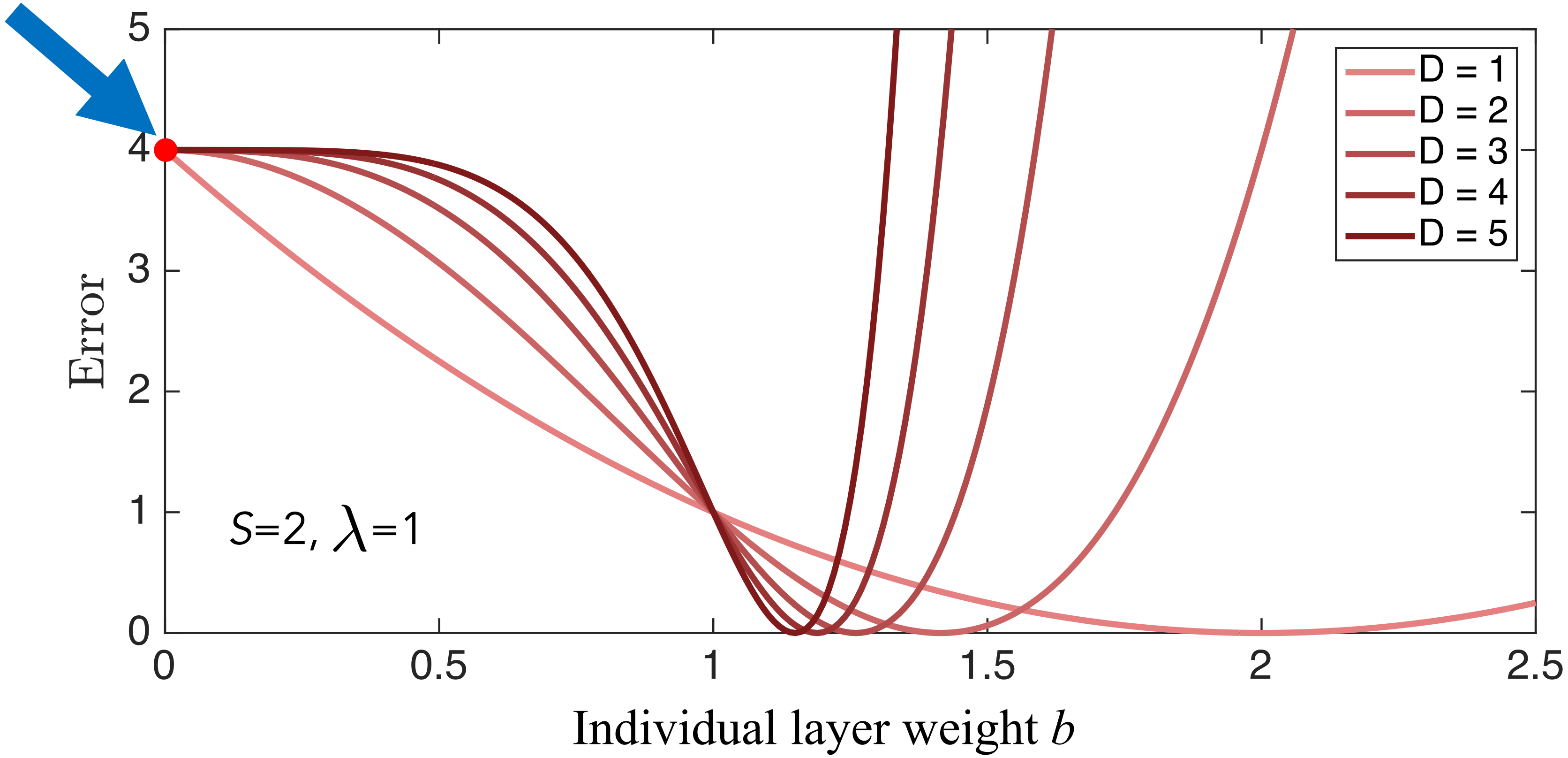
$$\tau \frac{d}{dt} W^l = \left(\prod_{i=l+1}^{D} W^i \right)^T \left[\Sigma^{yx} - \left(\prod_{i=1}^{D} W^i \right) \Sigma^{xx} \right] \left(\prod_{i=1}^{l-1} W^i \right)^T \qquad l = 1, \cdots, D$$

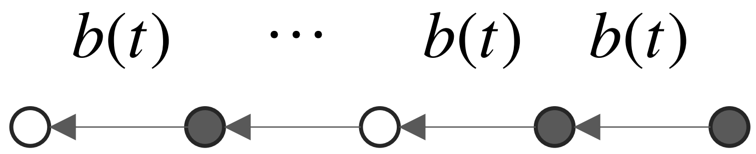
A linear chain



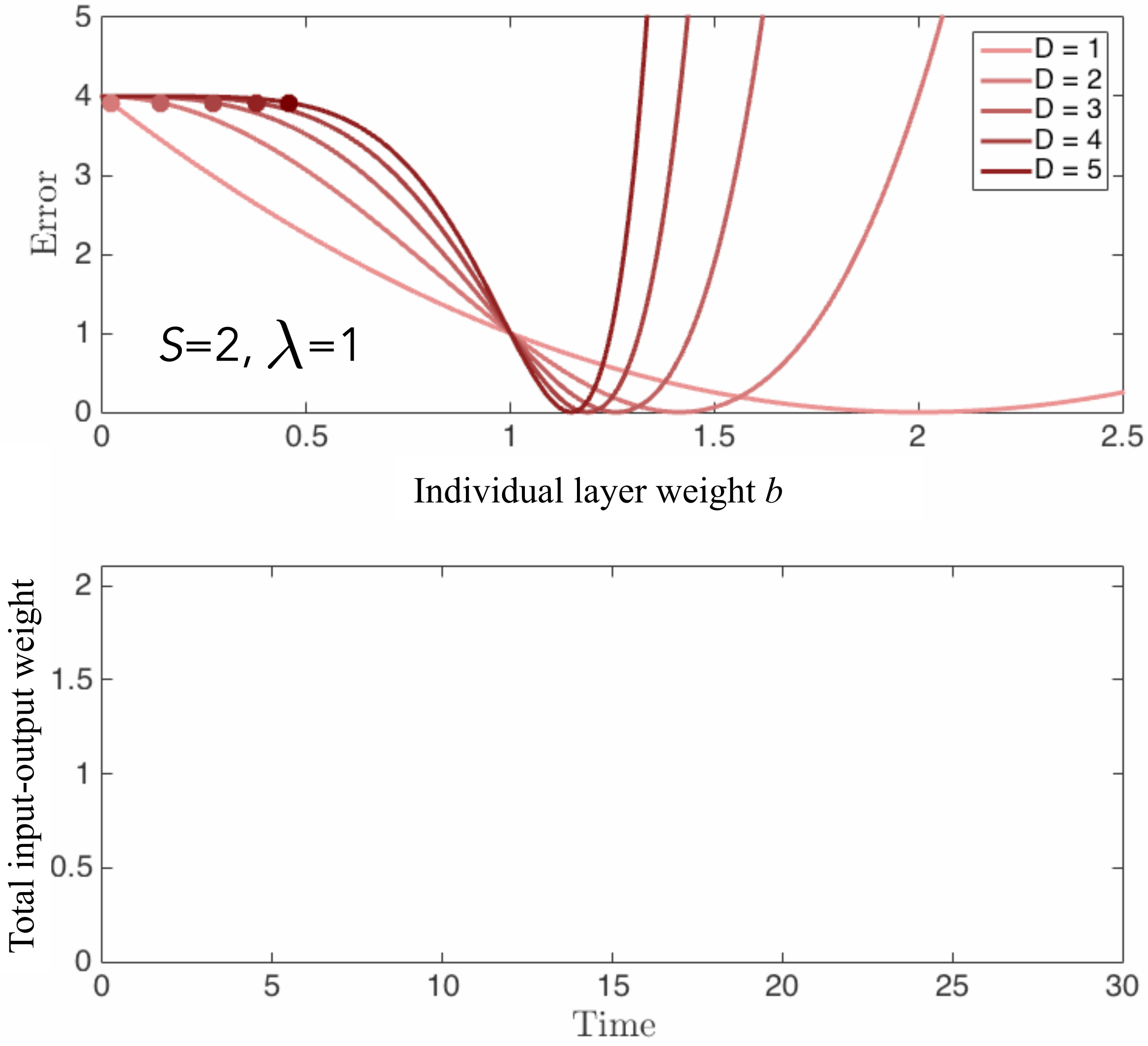
Error surface

Depth introduces a saddle point





Gradient descent dynamics



Analytic learning trajectory

Shallow (*D*=1): $$a(t) = \frac{s}{\lambda}\left(1 - e^{-t/\tau}\right) + a_0 e^{-t/\tau}$$

Deep (*D*=2): $$a(t) = \frac{s/\lambda}{1 - \left(1 - \frac{s}{\lambda a_0}\right) e^{-\frac{2st}{\tau}}}$$

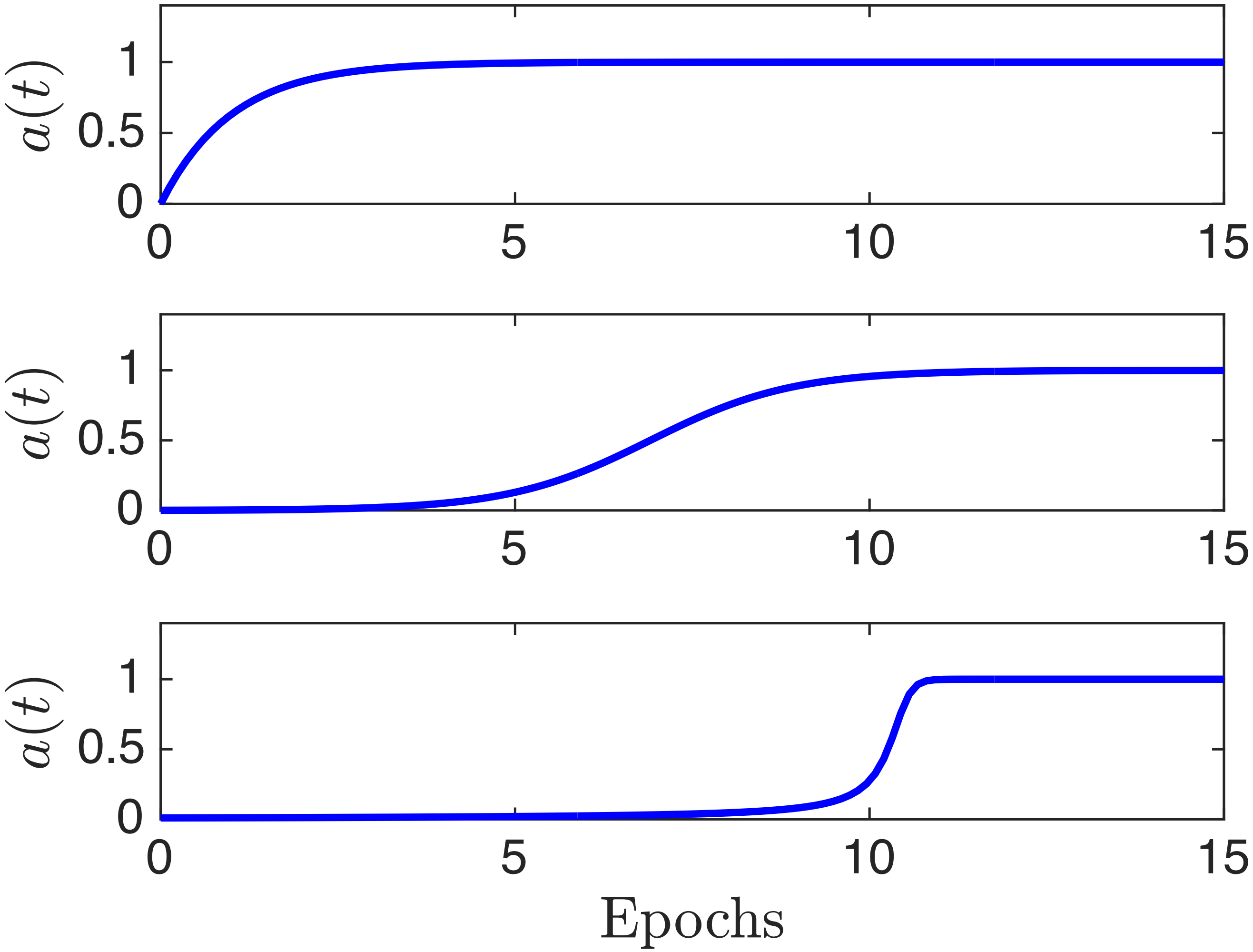
V. Deep (*D*$\longrightarrow\infty$): $$a(t) = \frac{s/\lambda}{1 + W\left[\left(\frac{s}{\lambda a_0} - 1\right) e^{\frac{s}{\lambda a_0} - 1 - t/\tau}\right]}$$

Analytic learning trajectory

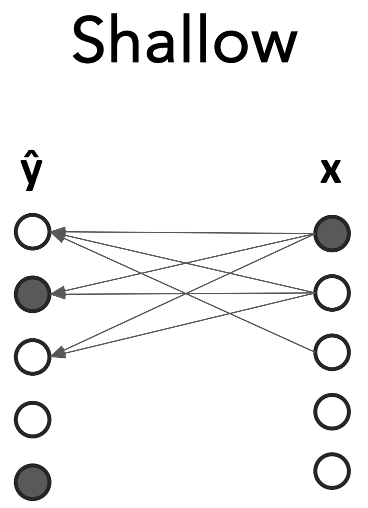
Shallow (D=1):

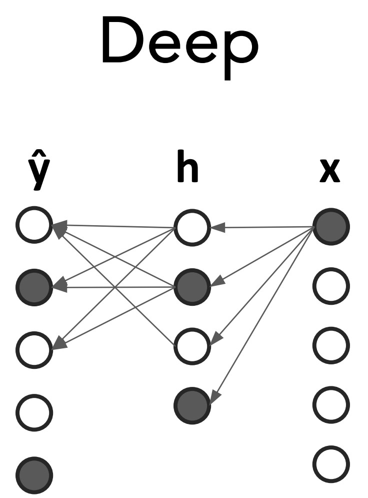
Deep (D=2):

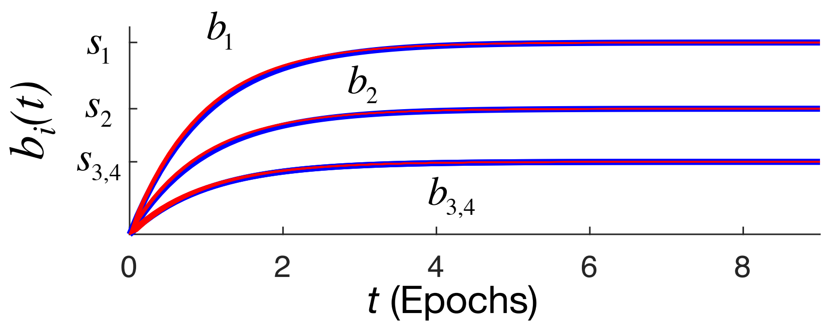
V. Deep ($D \longrightarrow \infty$):

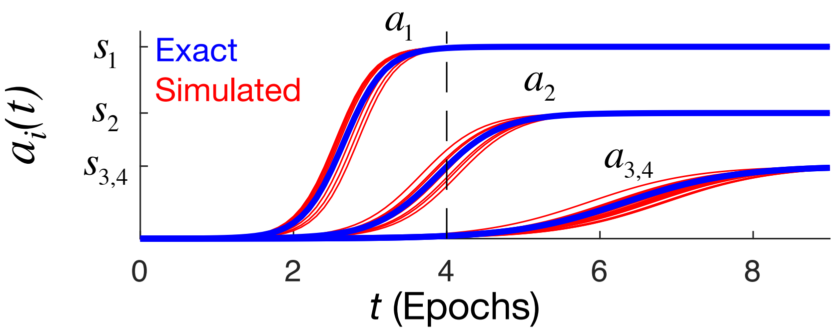


Full networks act like several 1D chains

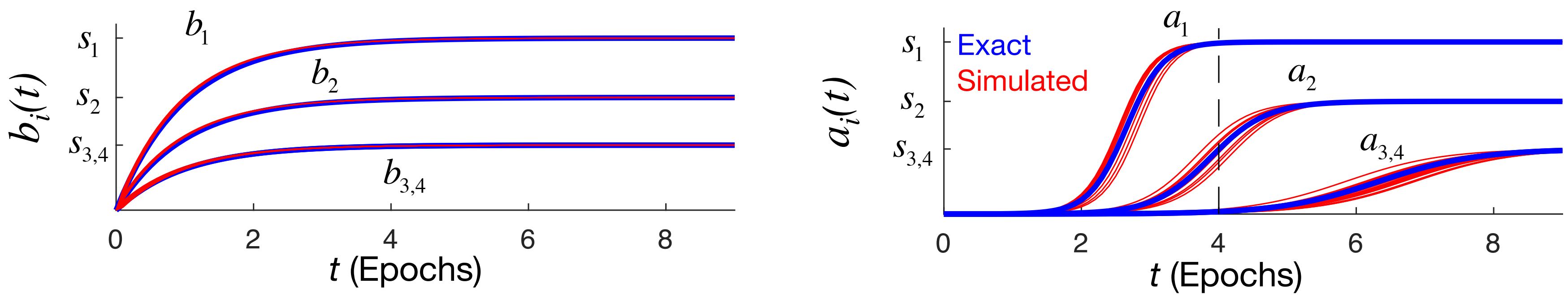








Depth introduces stage-like transitions



Training speed

- How does training speed scale with depth?

- Time difference for deep net vs shallow net is

$$t_\infty - t_1 \approx O\left(\frac{1}{s b_0^D}\right)$$

t_D	epochs to train depth D network
b_0	Initial layer singular value
s	Minimum nonzero singular value
D	Depth

- Deep learning speed is highly sensitive to initial conditions

Effect of initialization

- **Small random weights** scale exponentially

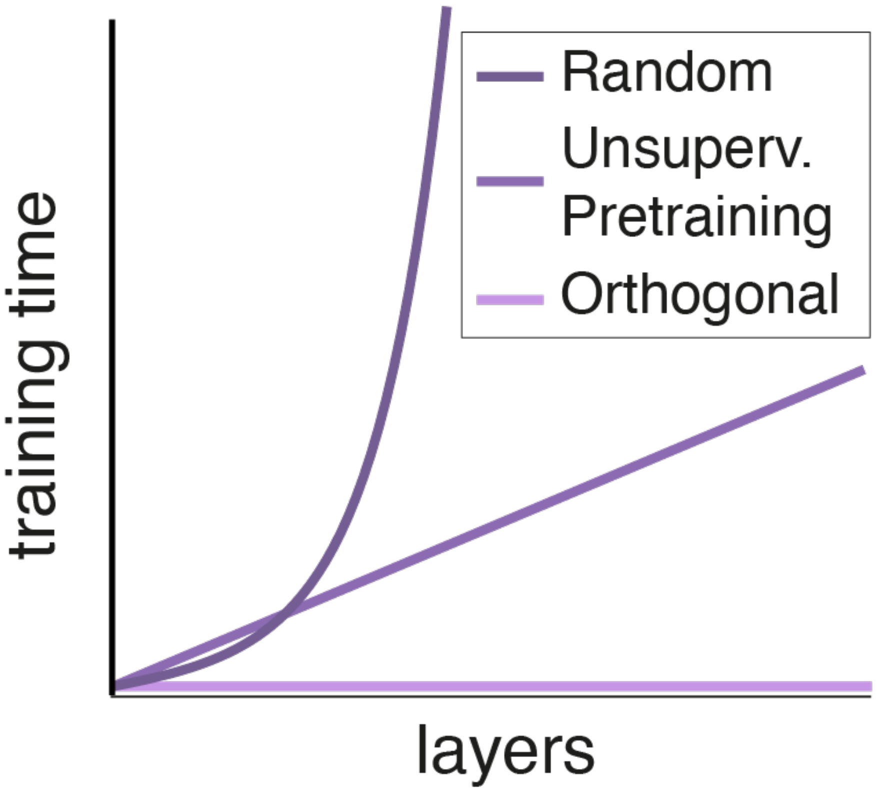
$$t_\infty - t_1 \approx O(1/b_0^D)$$

- **Pretraining + fine-tuning** scales linearly

$$t_\infty - t_1 \approx O(D/b_0^2)$$

- **Orthogonal initialization**: depth-independent

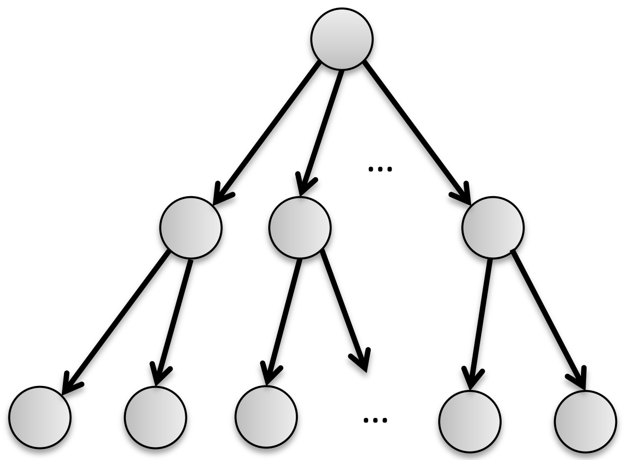
$$t_\infty - t_1 \approx O(1)$$



Connecting neural nets and graphical models

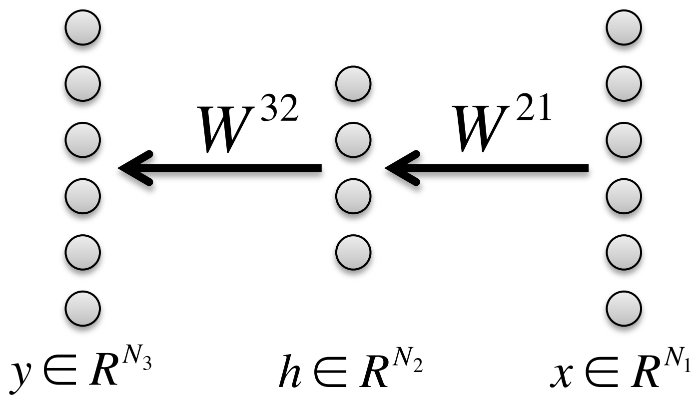
The "World":

Structured generative model



The "Learner":

Deep linear network



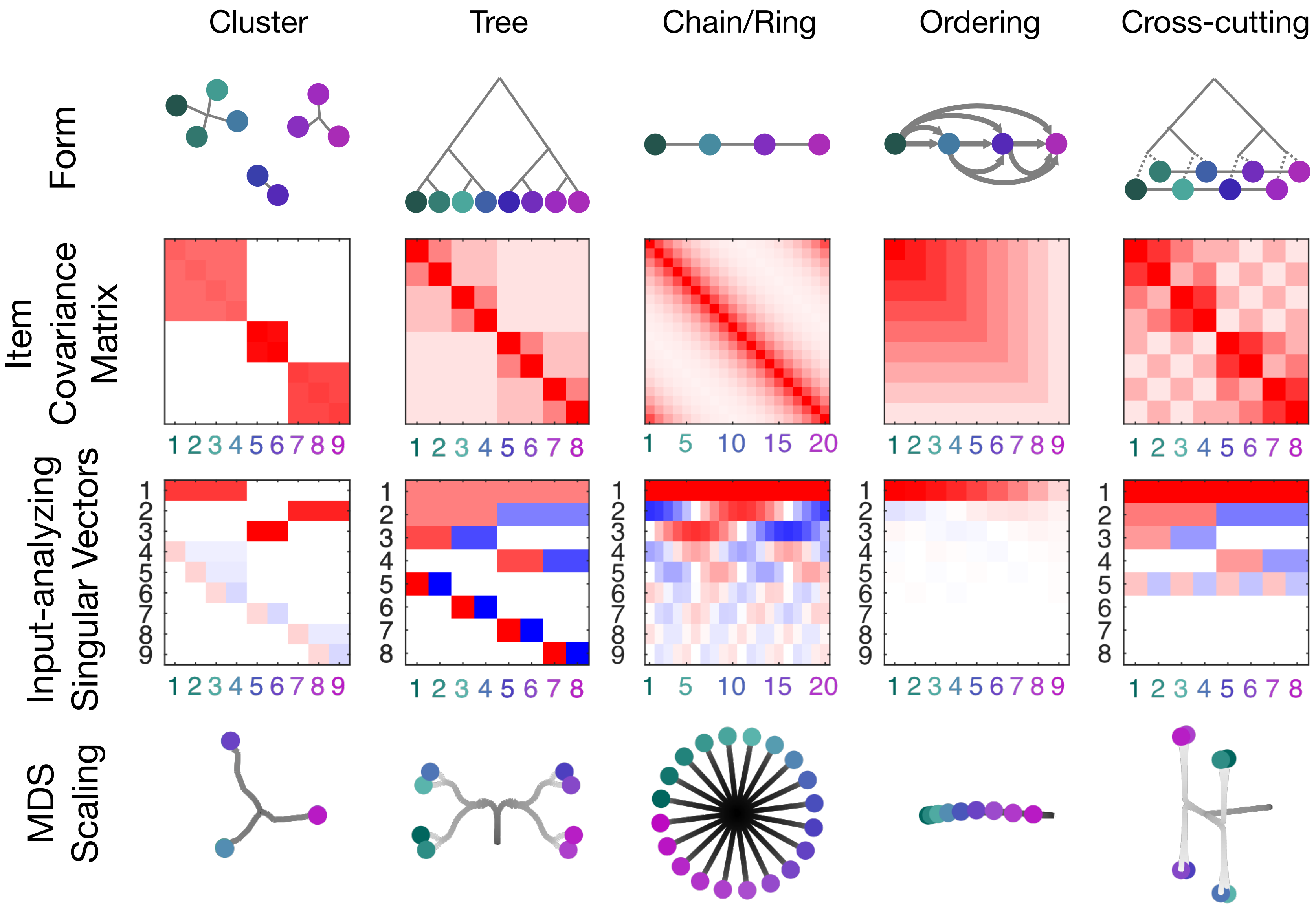
$$\{x^\mu, y^\mu\}, \mu = 1, \ldots, P.$$

Analytic link

- In the limit of many features, what matters to learning dynamics is SVD of correlation structure

- Can find this exactly for certain graphical models
  - Partitions
  - Trees
  - Grids/rings

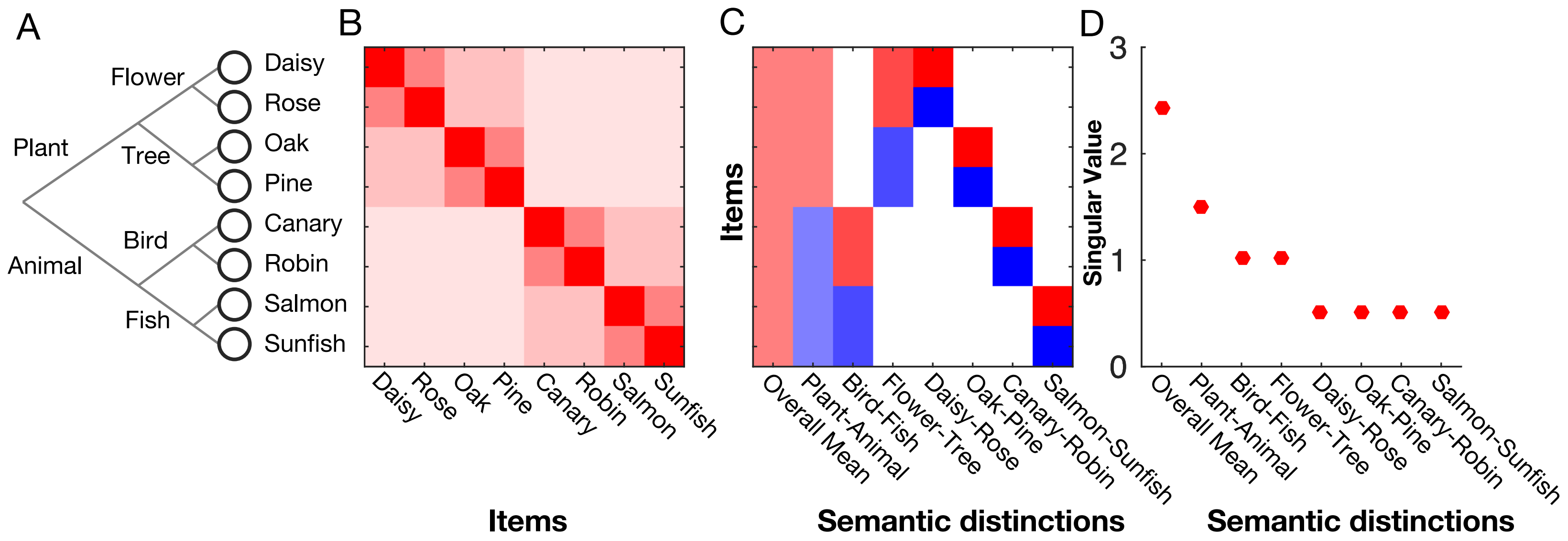
Learning diverse structures



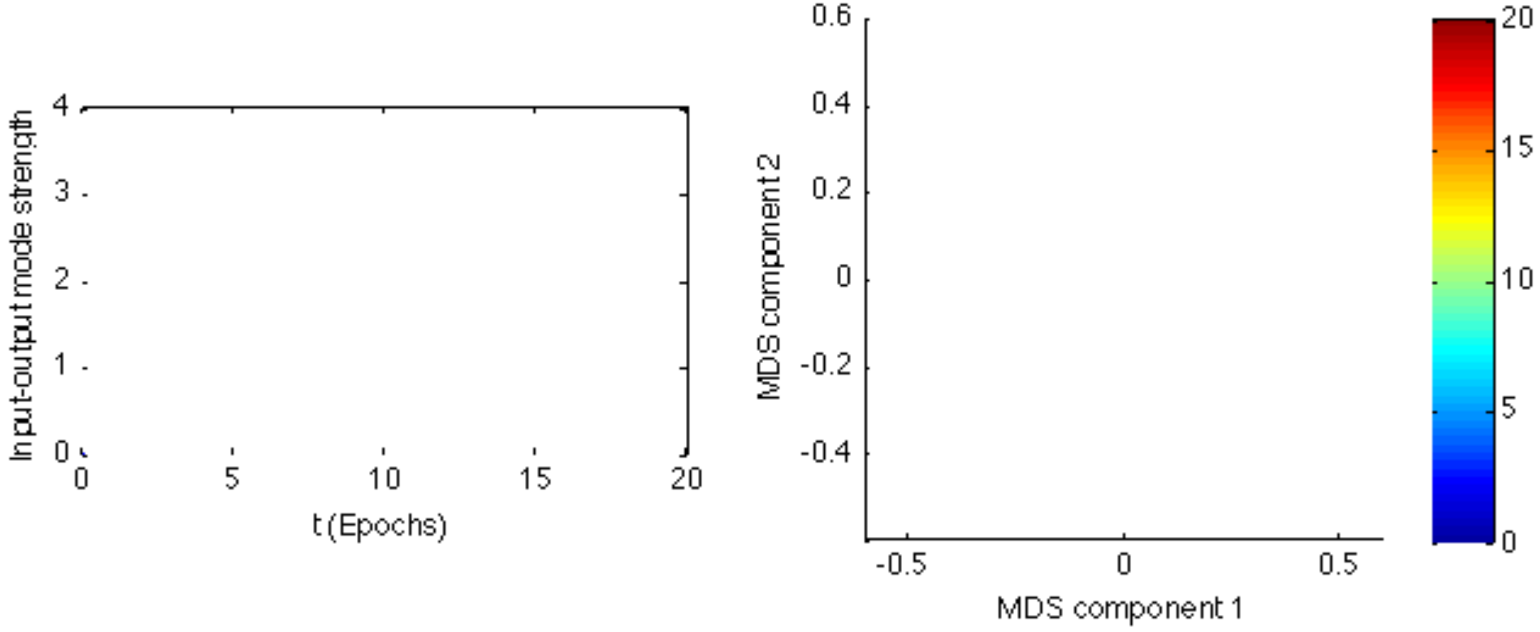
Progressive differentiation

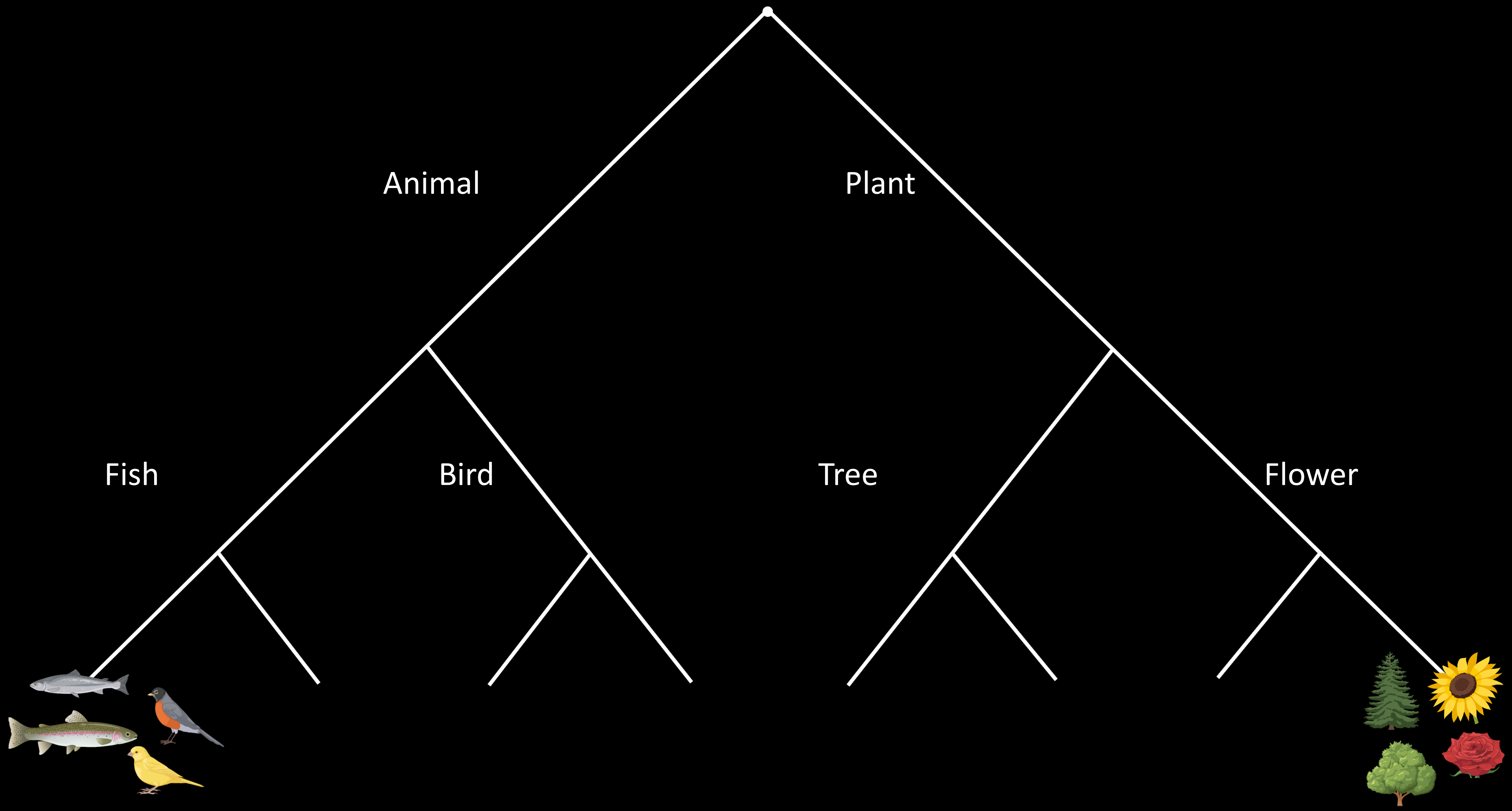
These networks **must** exhibit progressive differentiation:

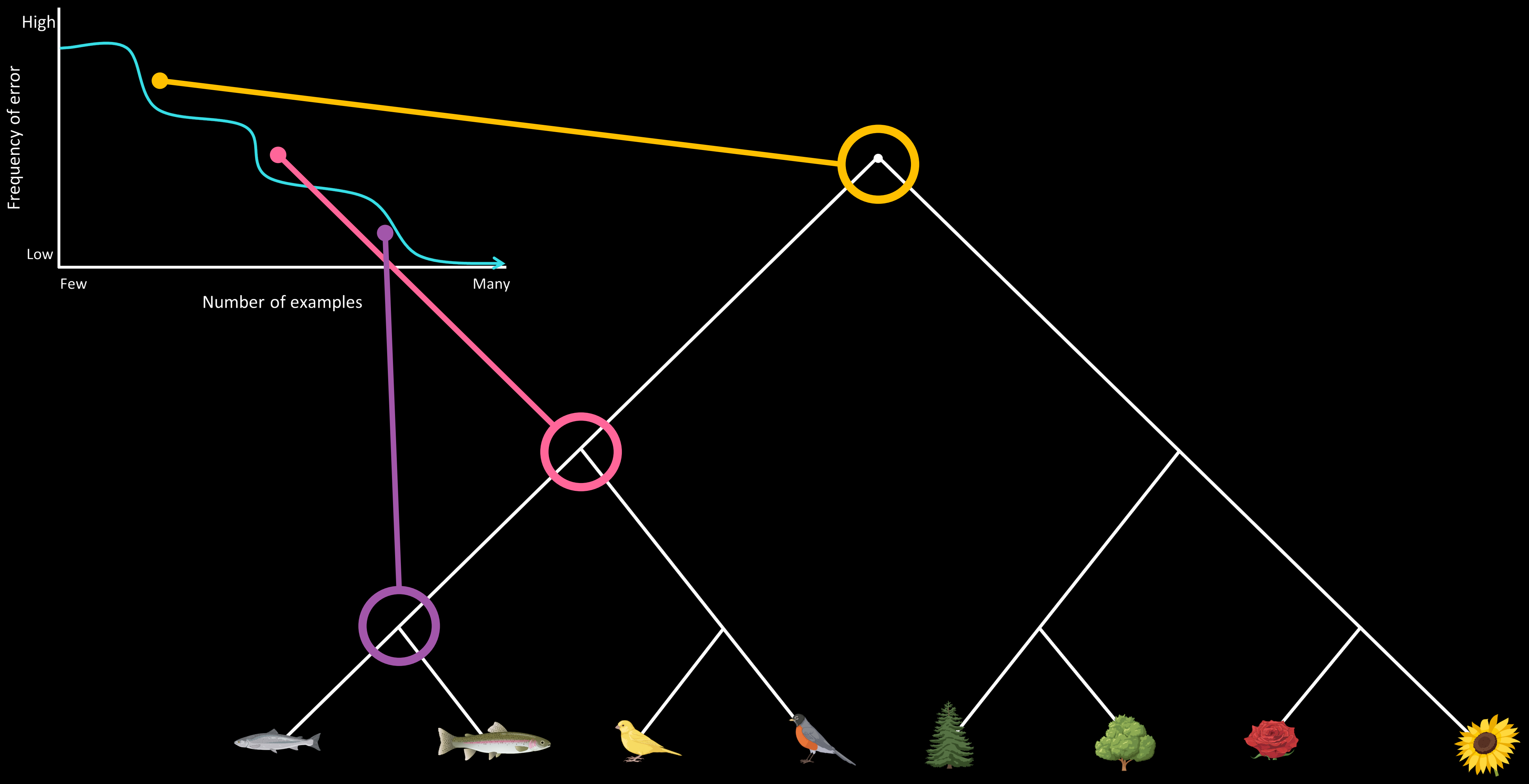
- Singular vectors mirror hierarchy
- Singular values decay with depth



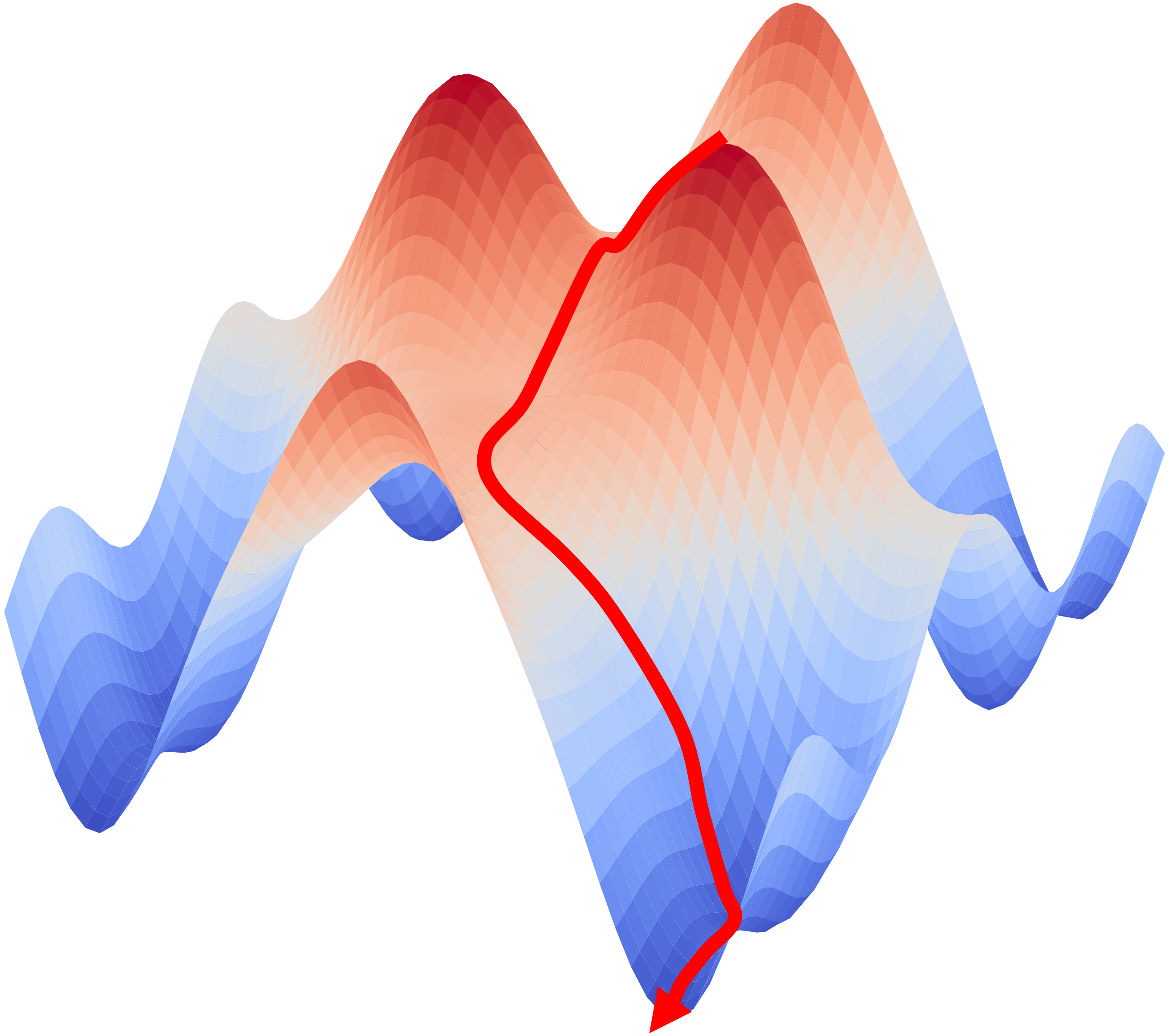
Progressive differentiation



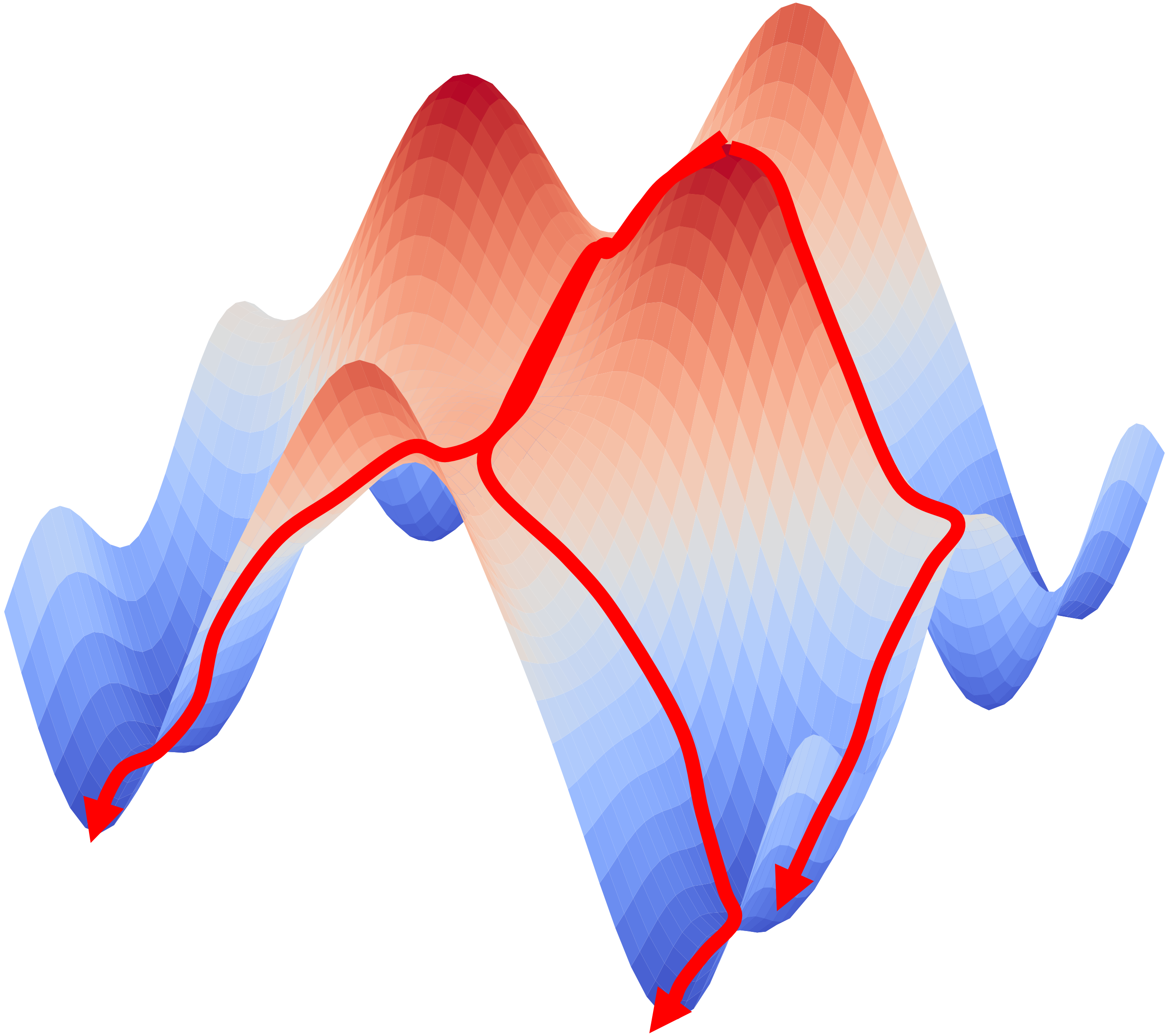

Animal
Plant
Fish
Bird
Tree
Flower


High
Frequency of error
Low
Few
Many
Number of examples

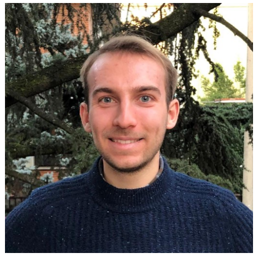
Depth introduces a hierarchy of saddle points



Individual variability amidst structure



Learning to make perceptual decisions from naïve to expert



Sam Liebana

Aeron Laffere

Chiara Toschi

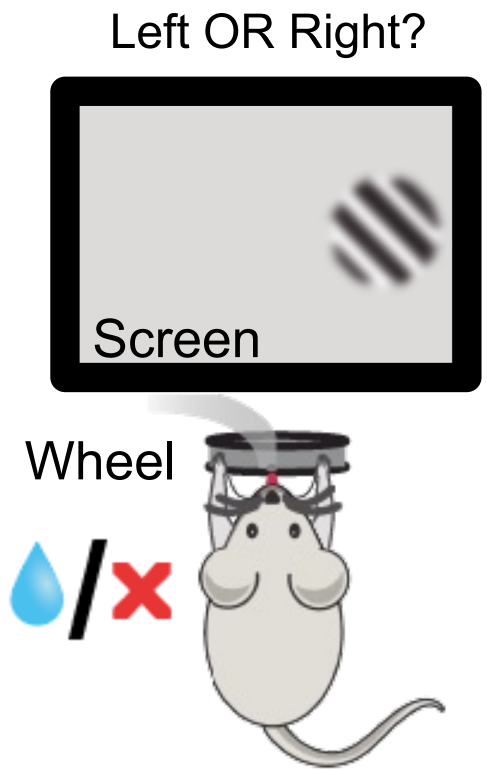
Peter Zatka-Haas

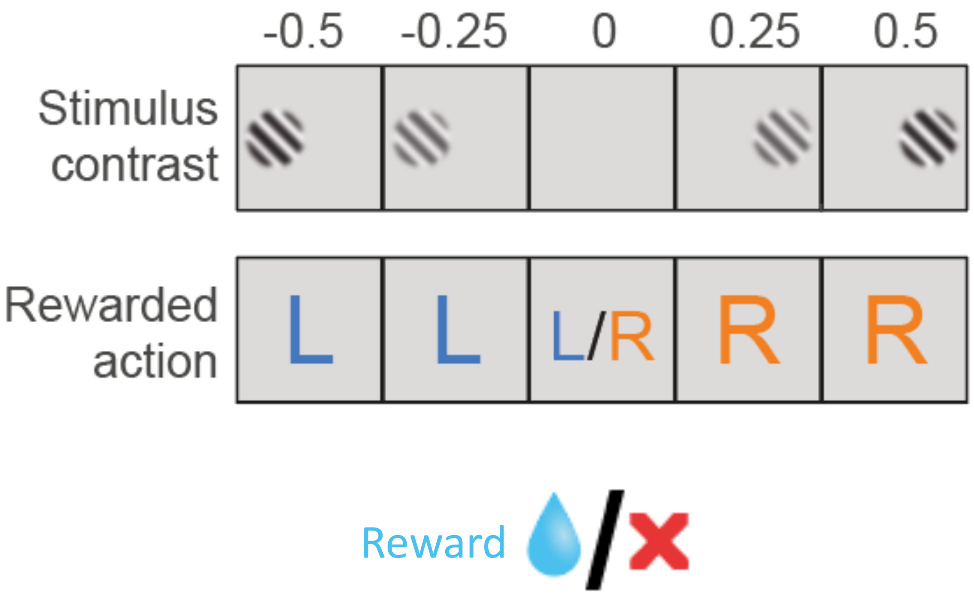
Louisa Schilling

Rafal Bogacz

Armin Lak

Learning to make perceptual decisions from naïve to expert

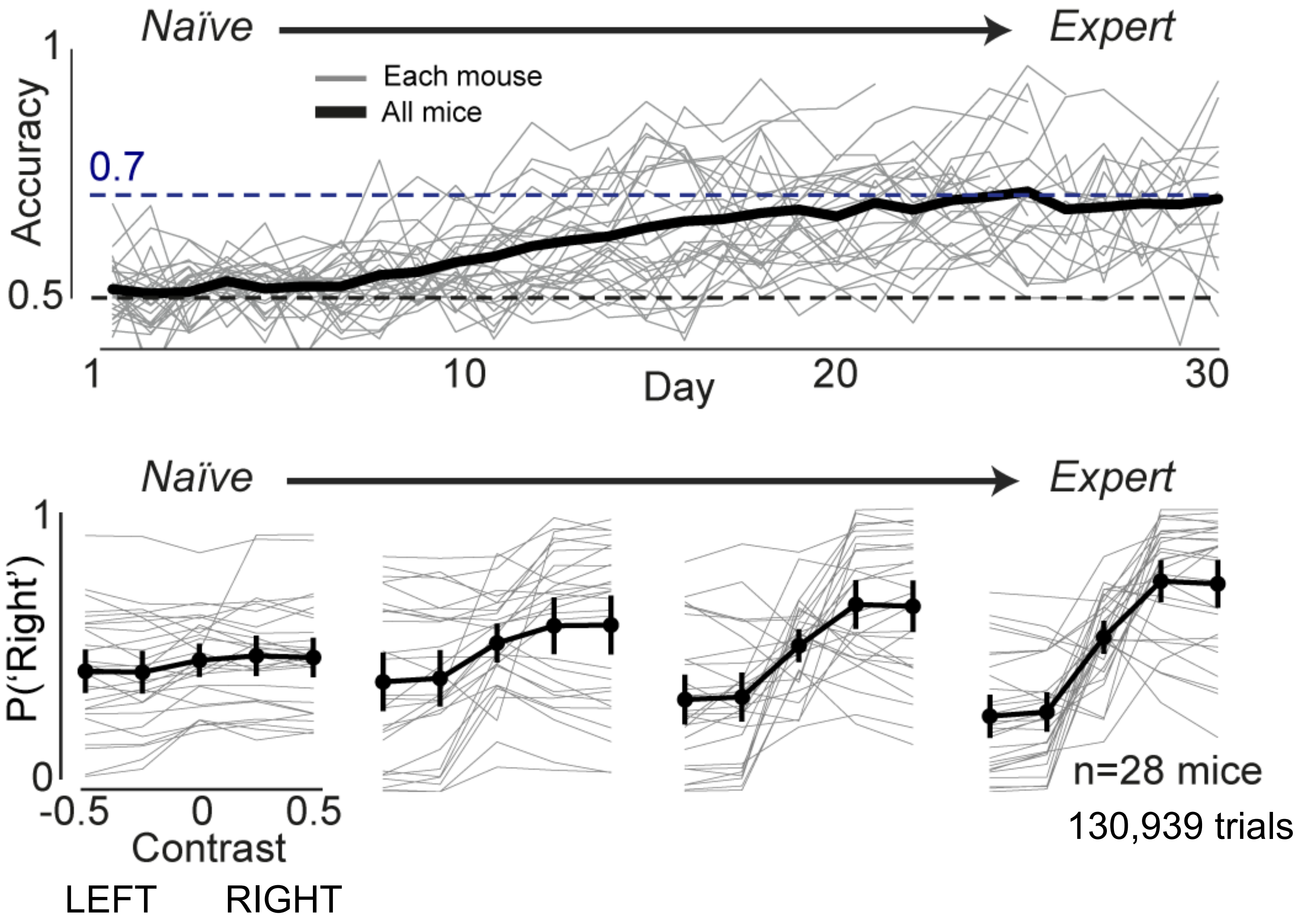




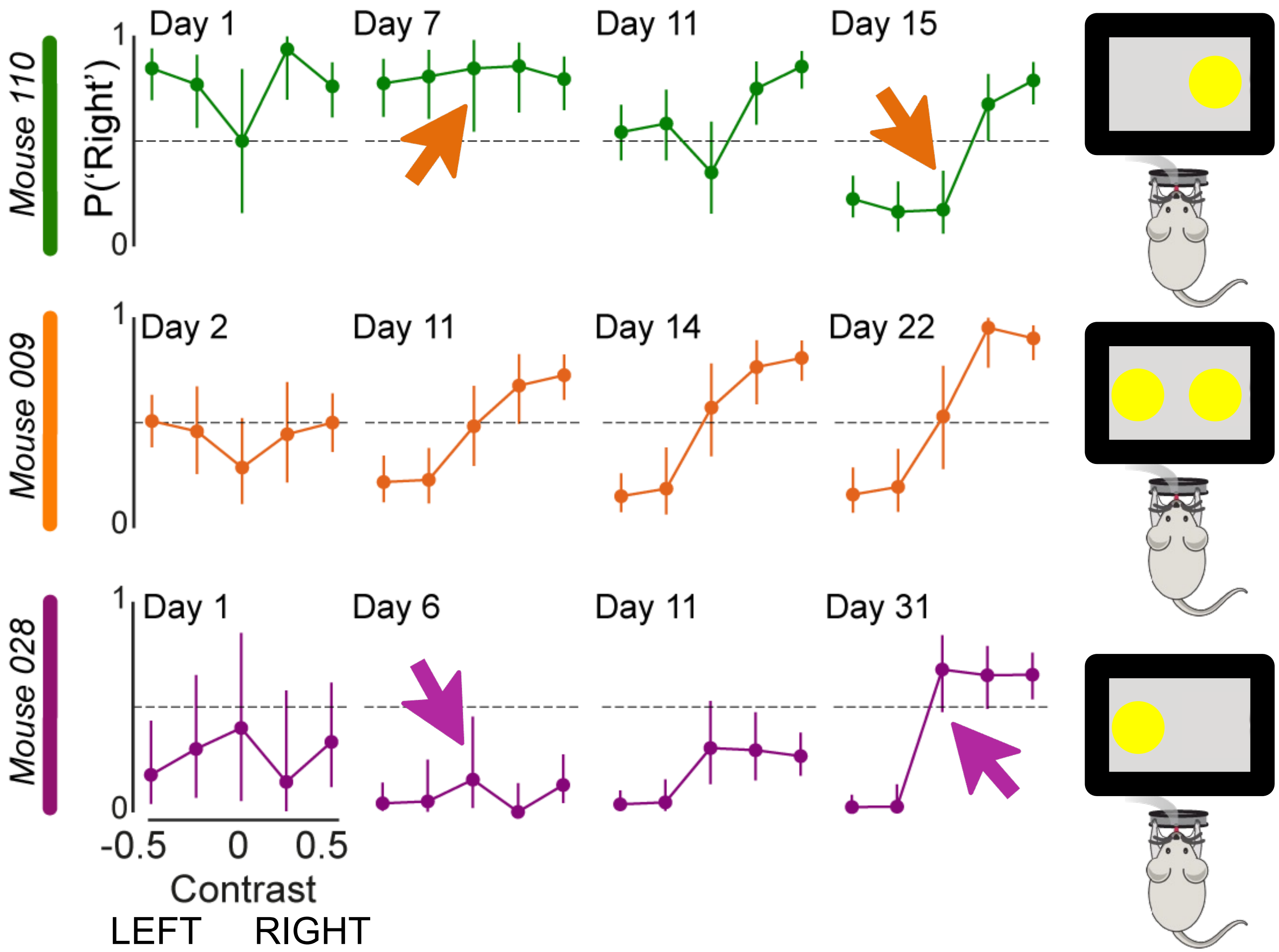
Full task from day 1 without any change over learning

Burgess, Lak*, Steinmetz*, Zatka-Haas* et al., Cell reports, 2017*

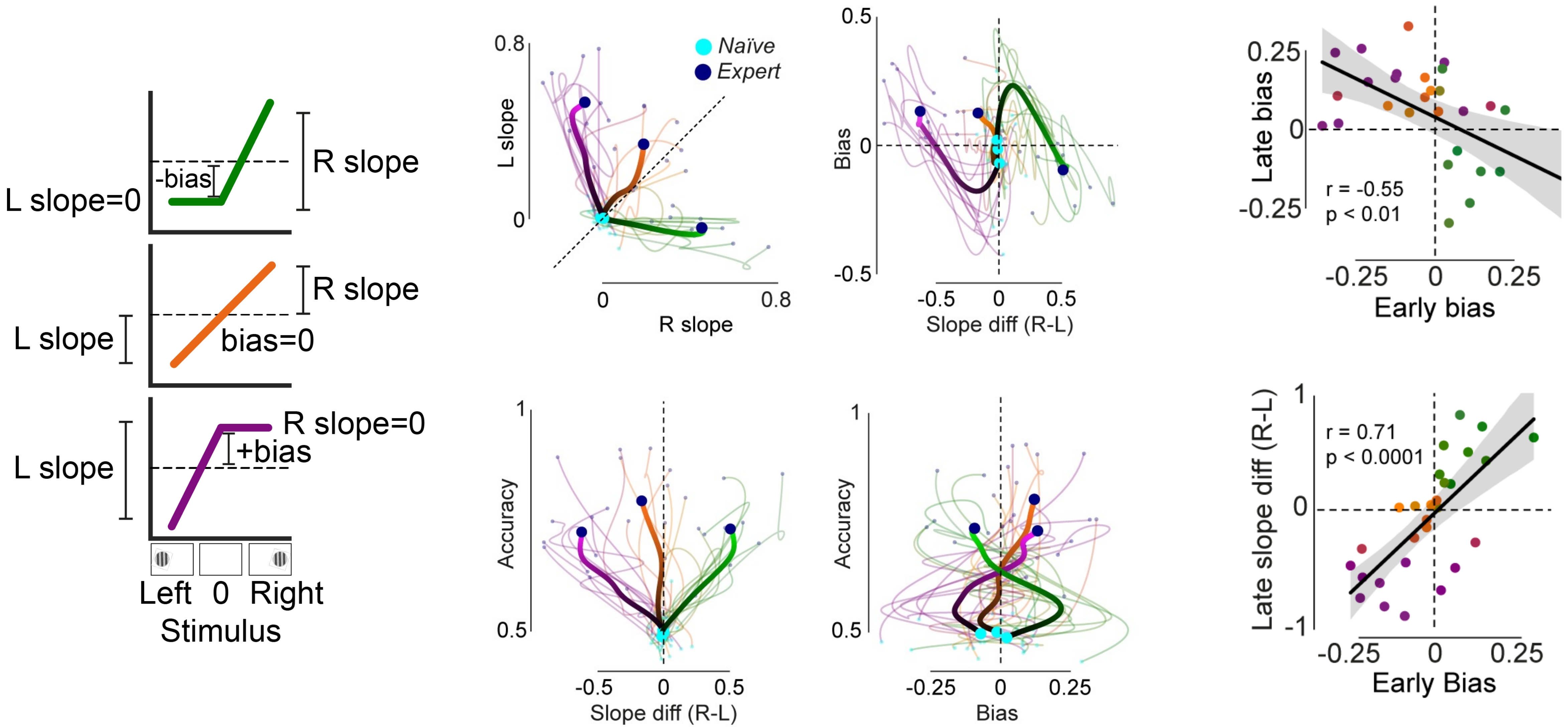
Learning to make perceptual decisions from naïve to expert



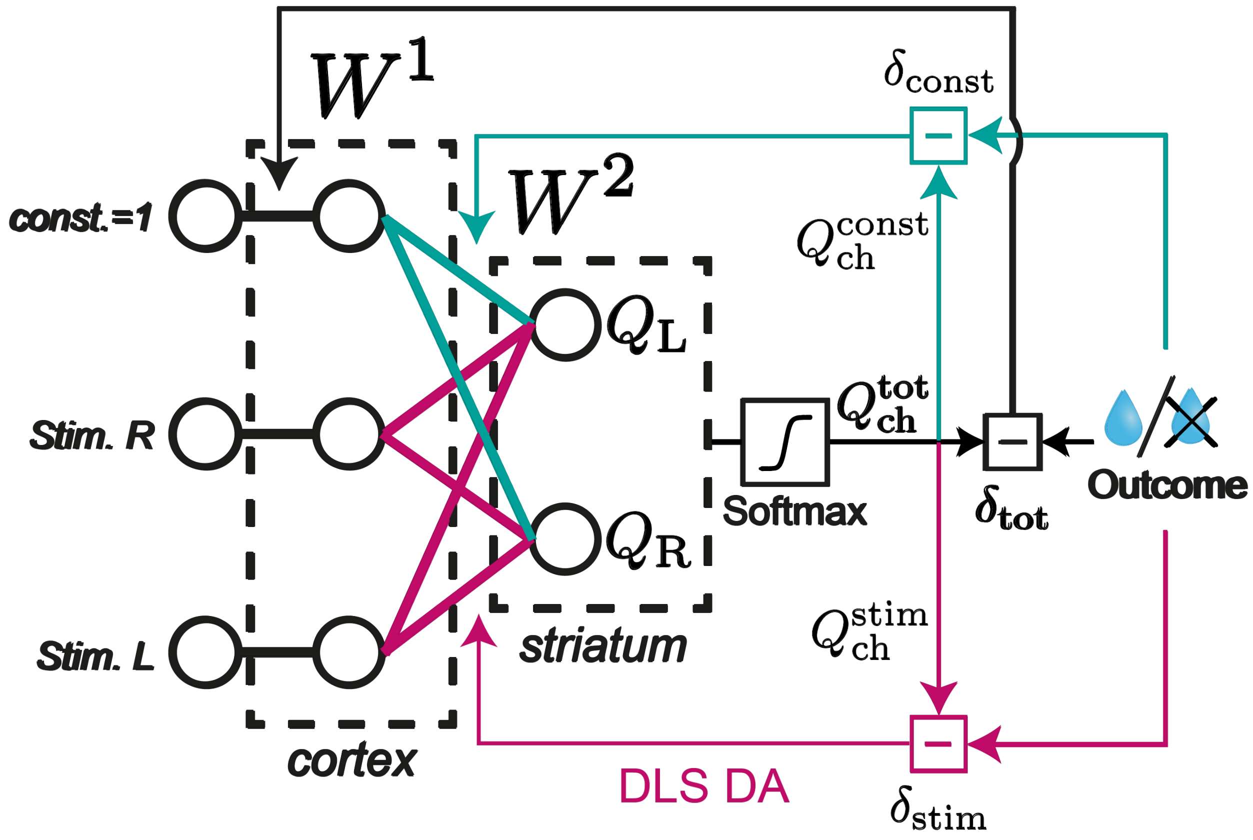
Mice exhibit diverse learning trajectories



Learning trajectories are individually diverse but systematic



A Deep RL Neural Network

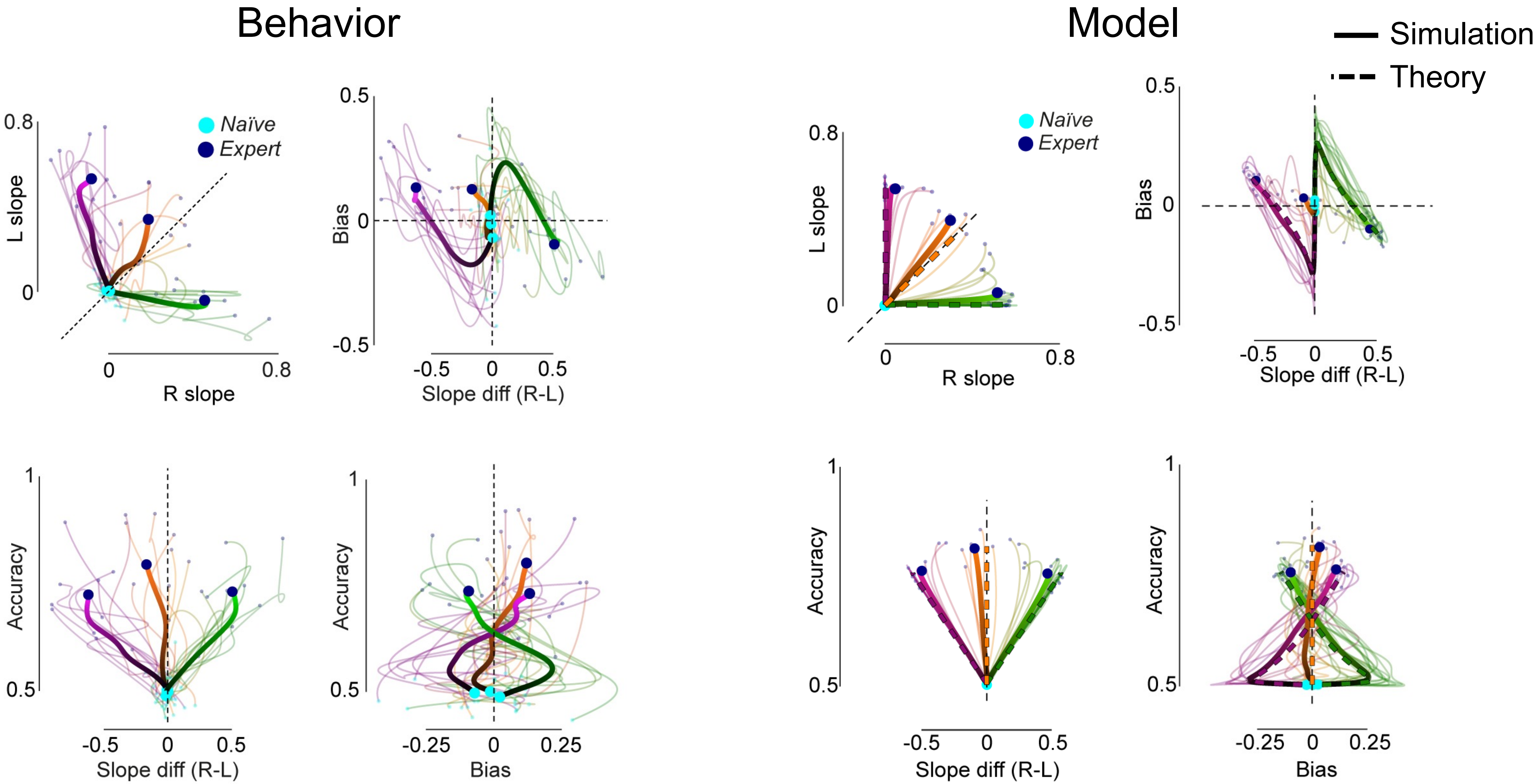


$$\mathcal{L}^{\text{cortex}} = \frac{1}{2}\delta^2_{\text{tot}} = \frac{1}{2}(\text{Rew} - Q^{\text{tot}}_{\text{ch}})^2$$

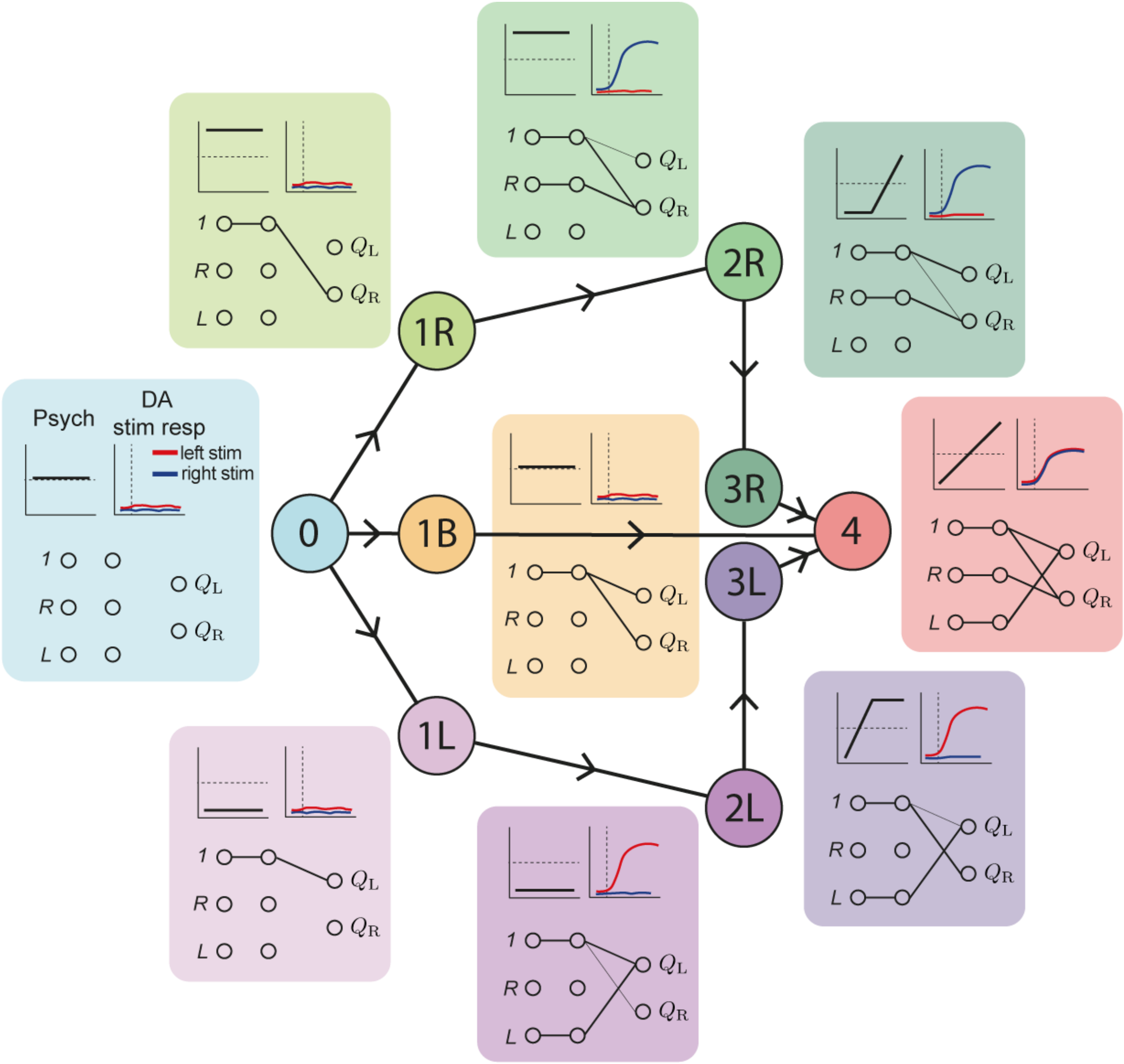
$$\mathcal{L}^{\text{const}} = \frac{1}{2}\delta^2_{\text{const}} = \frac{1}{2}(\text{Rew} - Q^{\text{const}}_{\text{ch}})^2$$

$$\mathcal{L}^{\text{stim}} = \frac{1}{2}\delta^2_{\text{stim}} = \frac{1}{2}(\text{Rew} - Q^{\text{stim}}_{\text{ch}})^2$$

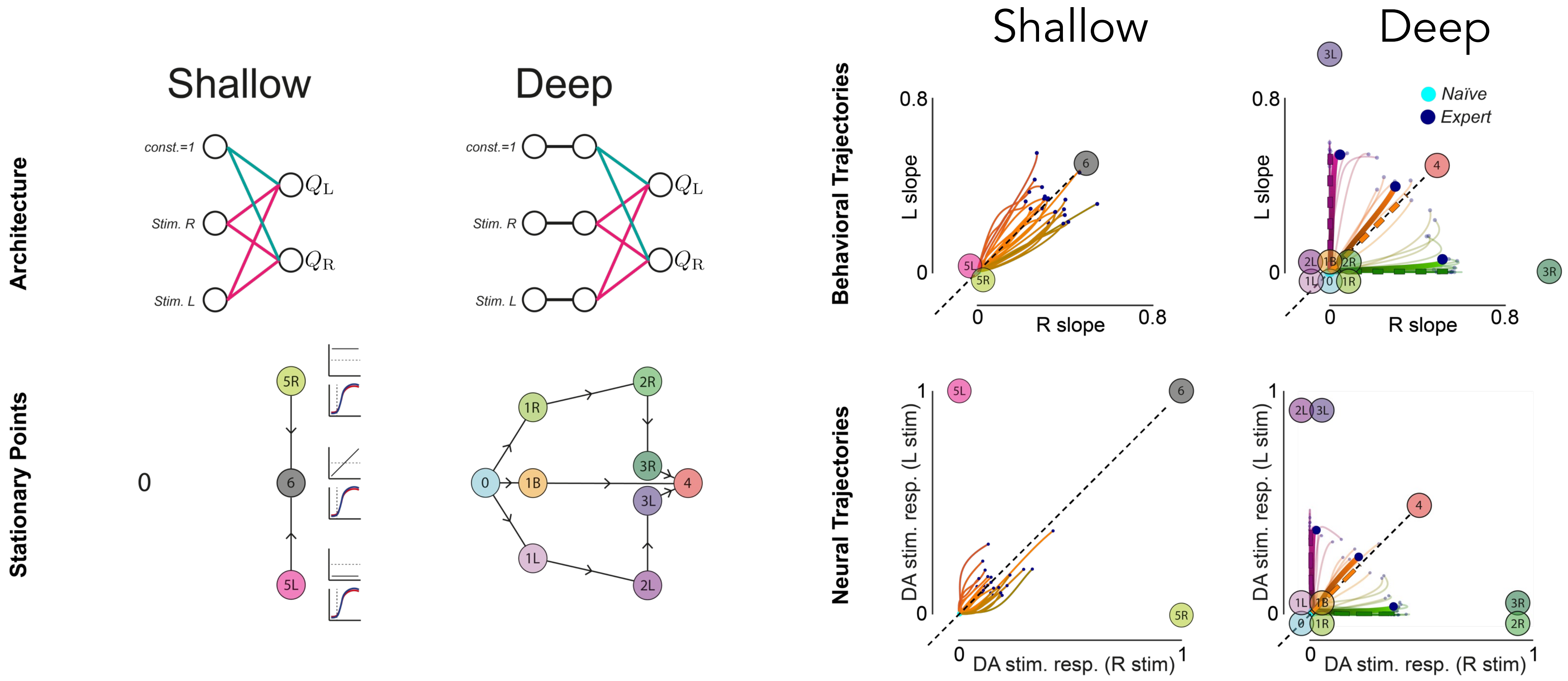
Model captures behavior



Dynamics pass near a hierarchy of saddle points



Saddle points arise through depth



Today

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2. Nontrivial initializations: Lazy, rich, & beyond

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Partitioned solution

$$\mathbf{QQ}^T(t) = \begin{pmatrix} \boldsymbol{Z_1}(t)\boldsymbol{A}^{-1}(t)\boldsymbol{Z_1^T}(t) & \boldsymbol{Z_1}(t)\boldsymbol{A}^{-1}(t)\boldsymbol{Z_2^T}(t) \\ \boldsymbol{Z_2}(t)\boldsymbol{A}^{-1}(t)\boldsymbol{Z_1^T}(t) & \boldsymbol{Z_2}(t)\boldsymbol{A}^{-1}(t)\boldsymbol{Z_2^T}(t) \end{pmatrix},$$

with the time-dependent variables $\boldsymbol{Z_1}(t) \in \mathbb{R}^{N_i \times N_h}$, $\boldsymbol{Z_2}(t) \in \mathbb{R}^{N_o \times N_h}$, *and* $\boldsymbol{A}(t) \in \mathbb{R}^{N_h \times N_h}$*:*

$$\boldsymbol{Z_1}(t) = \frac{1}{2}\tilde{\boldsymbol{V}}(\tilde{\boldsymbol{G}} - \tilde{\boldsymbol{H}}\tilde{\boldsymbol{G}})e^{\tilde{\boldsymbol{S}}_\lambda \frac{t}{\tau}}\boldsymbol{B}^T - \frac{1}{2}\tilde{\boldsymbol{V}}(\tilde{\boldsymbol{G}} + \tilde{\boldsymbol{H}}\tilde{\boldsymbol{G}})e^{-\tilde{\boldsymbol{S}}_\lambda \frac{t}{\tau}}\boldsymbol{C}^T + \tilde{\mathbf{V}}_\perp e^{\boldsymbol{\lambda}_\perp \frac{t}{\tau}}\boldsymbol{D}^T, \quad (13)$$

$$\boldsymbol{Z_2}(t) = \frac{1}{2}\tilde{\boldsymbol{U}}(\tilde{\boldsymbol{G}} + \tilde{\boldsymbol{H}}\tilde{\boldsymbol{G}})e^{\tilde{\boldsymbol{S}}_\lambda \frac{t}{\tau}}\boldsymbol{B}^T + \frac{1}{2}\tilde{\boldsymbol{U}}(\tilde{\boldsymbol{G}} - \tilde{\boldsymbol{H}}\tilde{\boldsymbol{G}})e^{-\tilde{\boldsymbol{S}}_\lambda \frac{t}{\tau}}\boldsymbol{C}^T + \tilde{\mathbf{U}}_\perp e^{\boldsymbol{\lambda}_\perp \frac{t}{\tau}}\boldsymbol{D}^T, \quad (14)$$

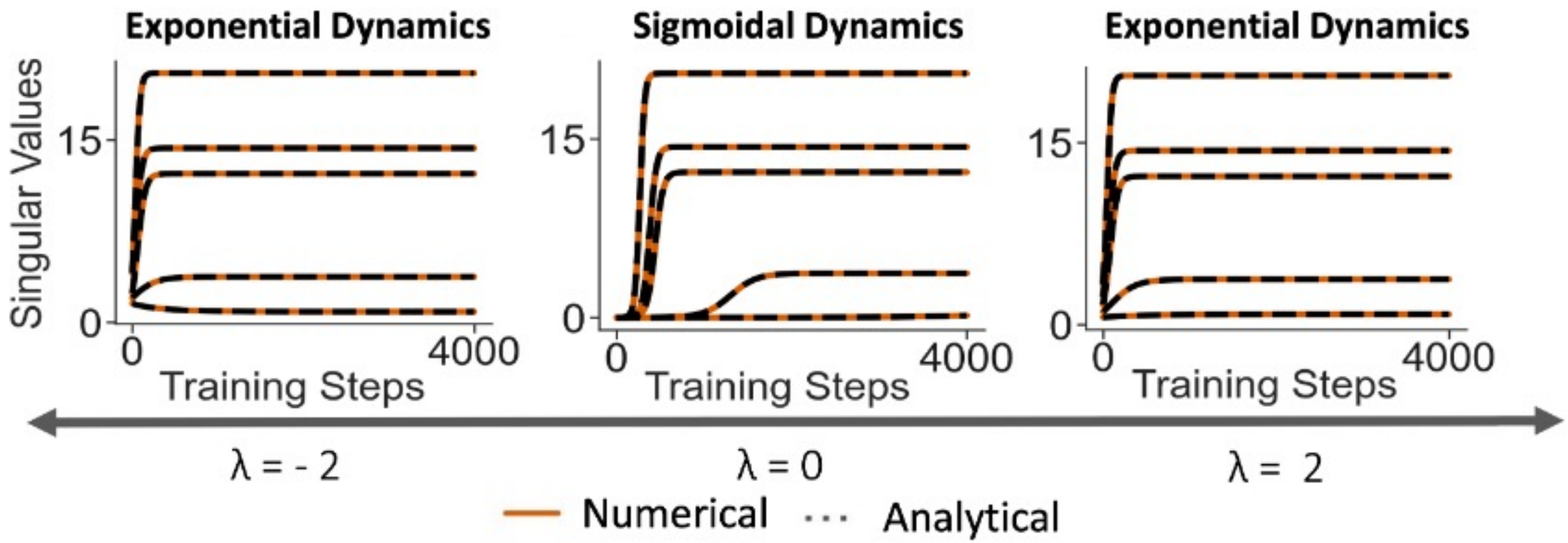
$$\boldsymbol{A}(t) = \mathbf{I} + \boldsymbol{B}\left(\frac{e^{2\tilde{\boldsymbol{S}}_\lambda \frac{t}{\tau}} - \mathbf{I}}{4\tilde{\boldsymbol{S}}_\lambda}\right)\boldsymbol{B}^T - \boldsymbol{C}\left(\frac{e^{-2\tilde{\boldsymbol{S}}_\lambda \frac{t}{\tau}} - \mathbf{I}}{4\tilde{\boldsymbol{S}}_\lambda}\right)\boldsymbol{C}^T + \boldsymbol{D}\left(\frac{e^{\boldsymbol{\lambda}_\perp \frac{t}{\tau}} - \mathbf{I}}{\boldsymbol{\lambda}_\perp}\right)\boldsymbol{D}^T. \quad (15)$$

and

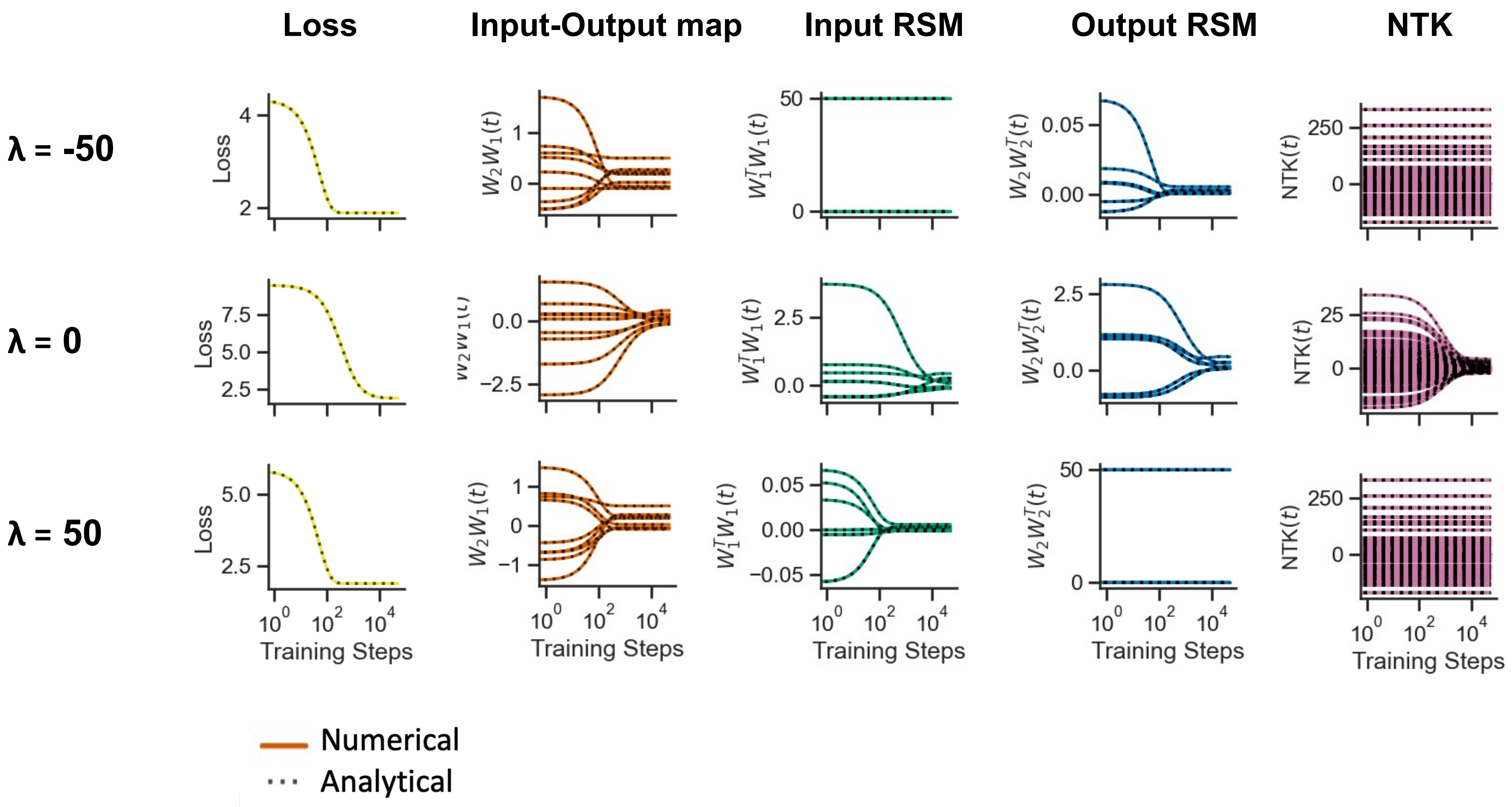
$$\tilde{\boldsymbol{S}}_\lambda = \sqrt{\tilde{\boldsymbol{S}}^2 + \frac{\lambda^2}{4}\mathbf{I}}, \quad \boldsymbol{\lambda}_\perp = \operatorname{sgn}(N_o - N_i)\frac{\lambda}{2}\mathbf{I}_{|N_o - N_i|}, \quad \tilde{\boldsymbol{H}} = \operatorname{sgn}(\lambda)\sqrt{\frac{\tilde{\boldsymbol{S}}_{\boldsymbol{\lambda}} - \tilde{\boldsymbol{S}}}{\tilde{\boldsymbol{S}}_{\boldsymbol{\lambda}} + \tilde{\boldsymbol{S}}}}, \quad \tilde{\boldsymbol{G}} = \frac{1}{\sqrt{\mathbf{I} + \tilde{\boldsymbol{H}}^2}}.$$

*where **B**, **C**, **D** are initialization-dependent matrices.*

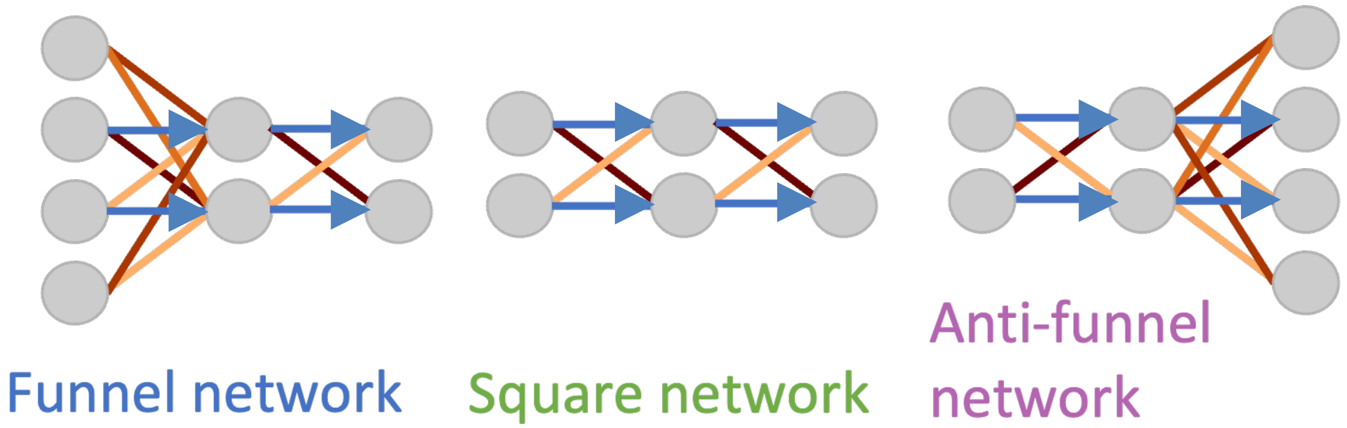
From exponential to sigmoidal dynamics

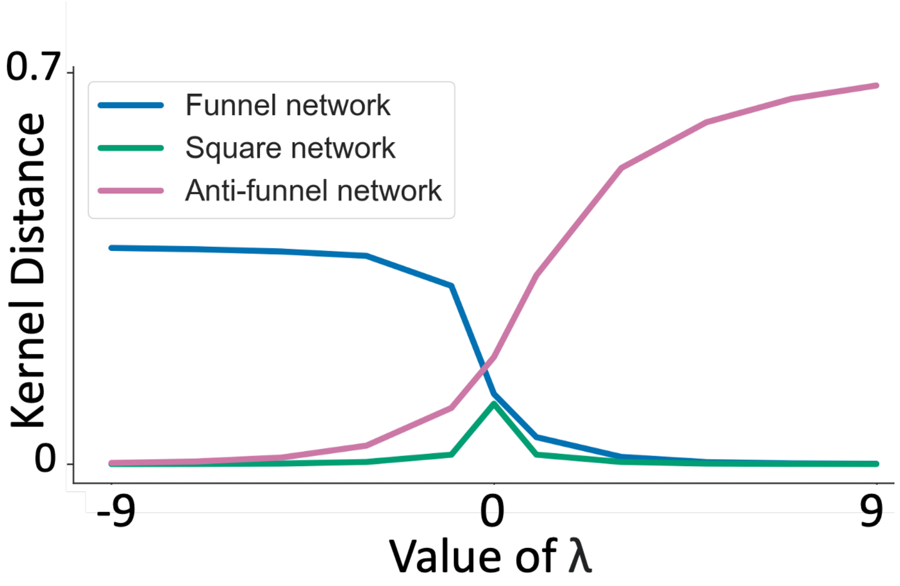


Rich and lazy learning



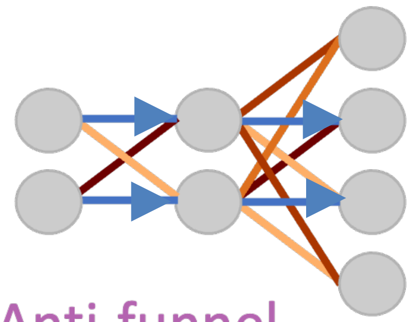
Architecture and learning regime



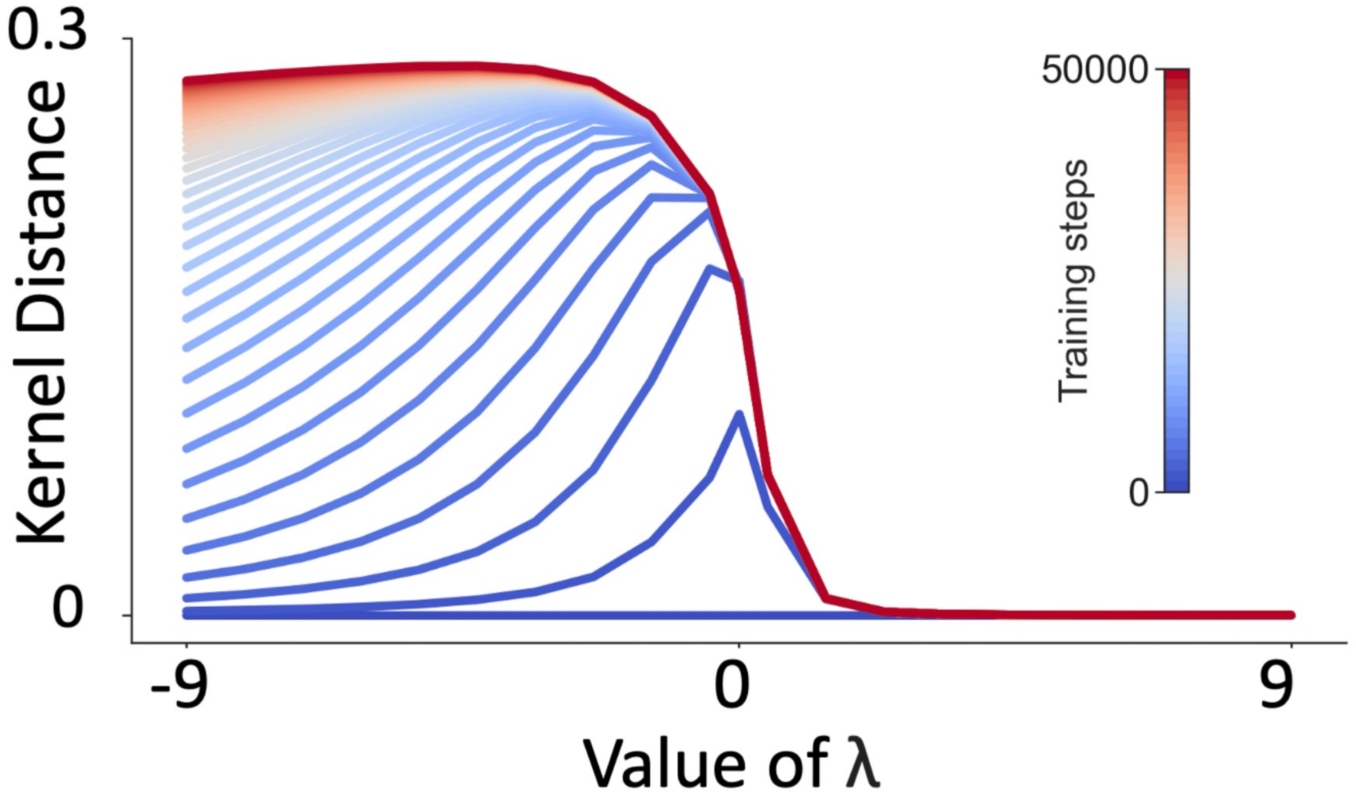


[Dominé and Anguita et al. 2024]

Delayed rich regime

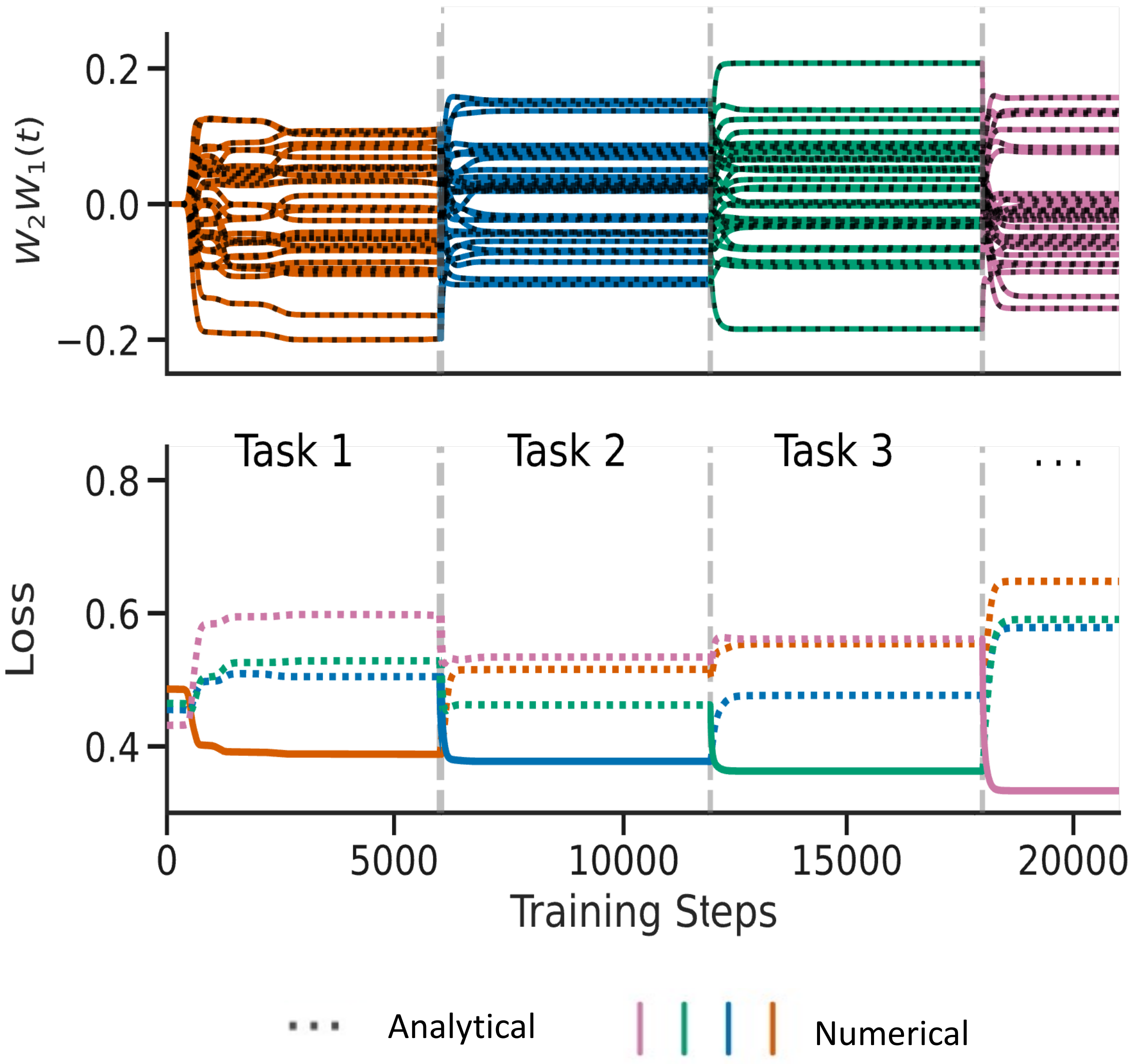


Anti-funnel network



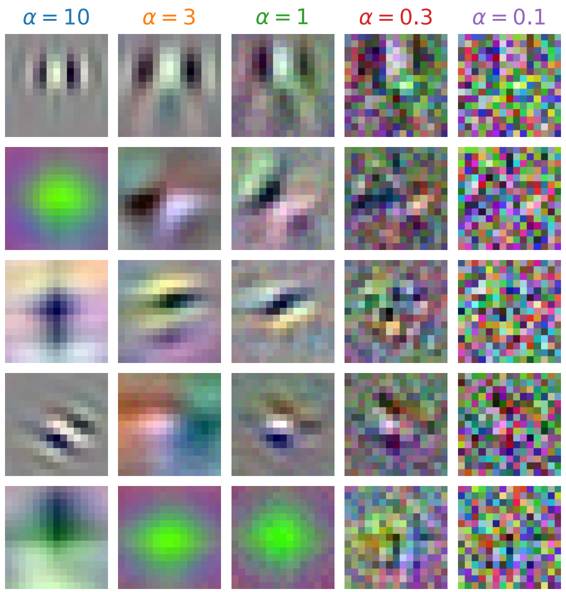
[Dominé and Anguita et al. 2024]

Exact continual learning dynamics

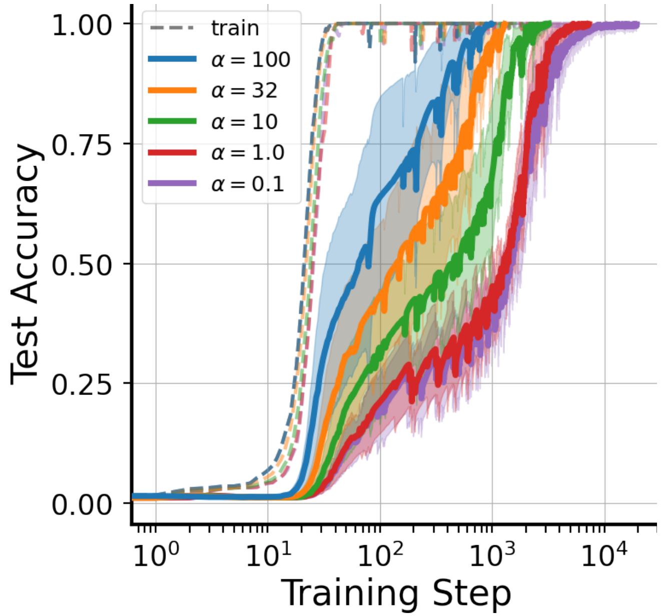


[Braun and Dominé et al. 2022, Dominé and Anguita et al. 2024]

Impact of relative scale initializations in practice



Promotes interpretability of early layers in CNNs



Decreases the time to grokking in modular arithmetic

Kunin et al. 2024

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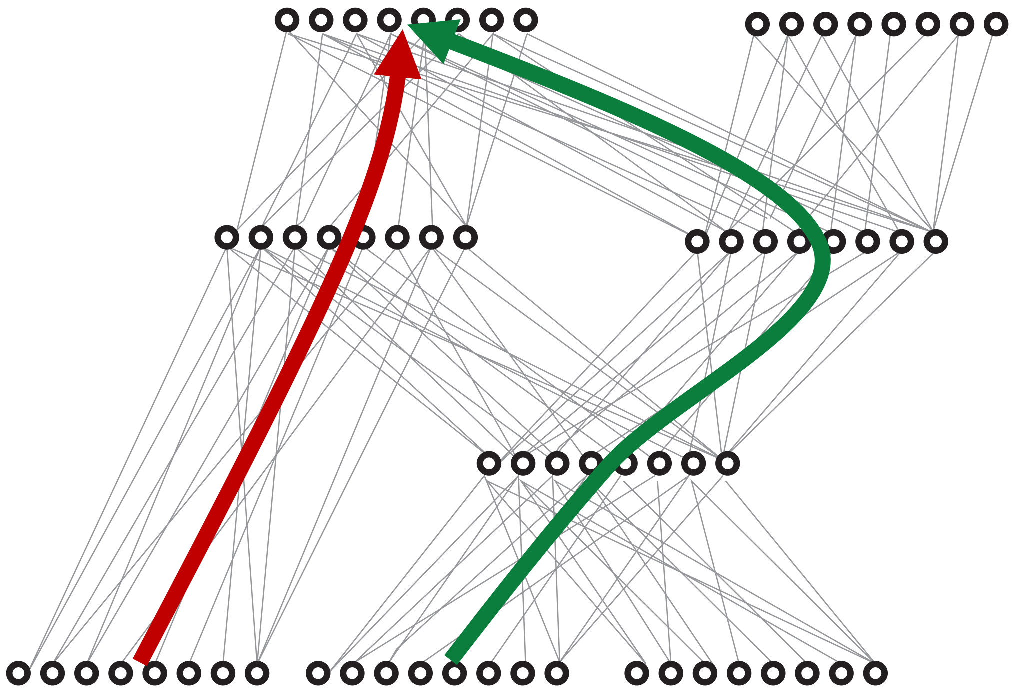
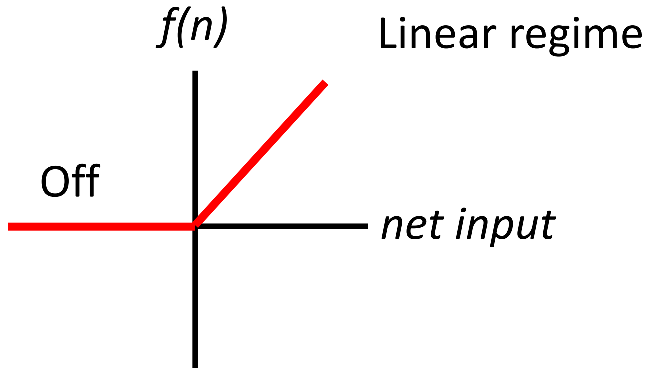
Gating: a simple view of nonlinearity



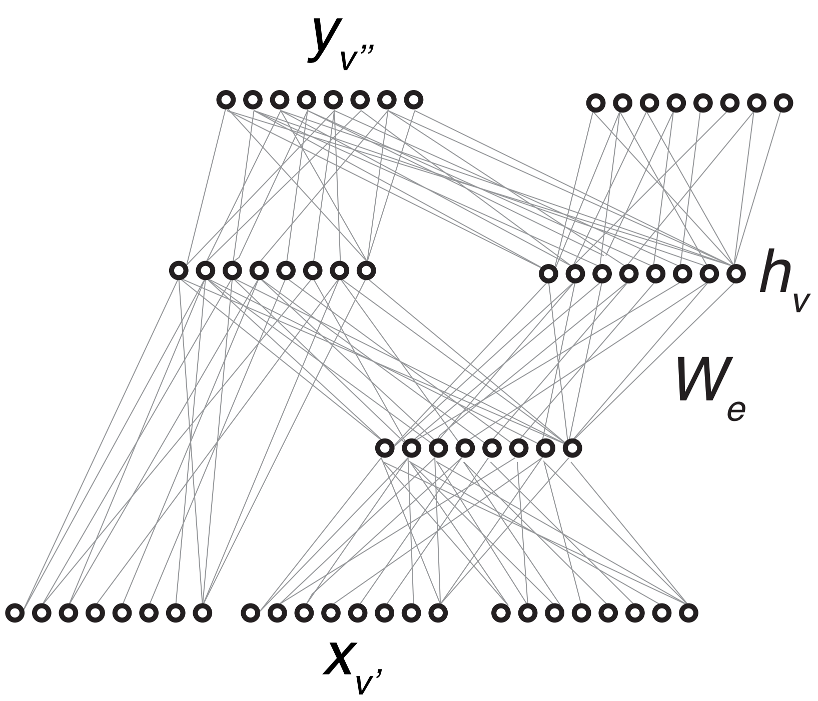
ReLU neural nonlinearity



When active, each pathway behaves like a deep linear network

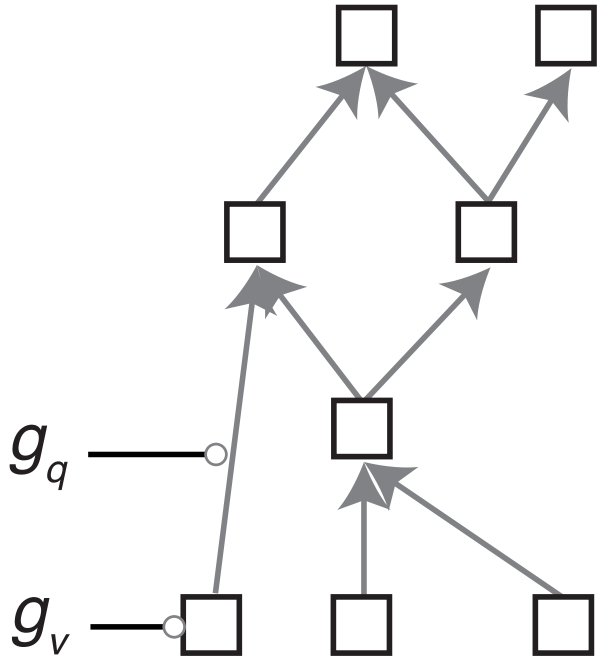
Lippl et al., 2022; Saxe et al., 2022; Li & Sompolinsky, 2022

Gated Deep Linear Network



Arch graph Γ: nodes V, edges E

Gated Deep Linear Network



Forward propagation:

$$h_v = g_v \sum_{q \in E : t(q) = v} g_q W_q h_{s(q)}$$

$s(q)$: source node of edge q
$t(q)$: target node of edge q

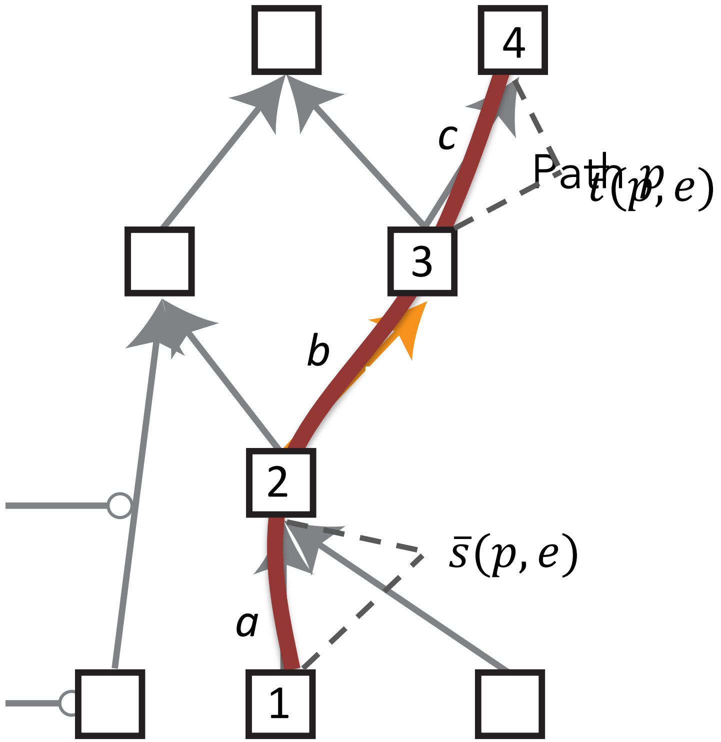
Gradient descent

Minimize L_2 loss $$\mathcal{L}(\{W\}) = \left\langle \frac{1}{2} \sum_{v \in \mathrm{Out}(\Gamma)} ||y_v - h_v||_2^2 \right\rangle_{x,y,g}$$

using gradient flow on the weights

$$\tau \frac{d}{dt} W_e = -\frac{\partial \mathcal{L}(\{W\})}{\partial W_e} \quad \forall e \in E$$

Gradient descent



Path notation

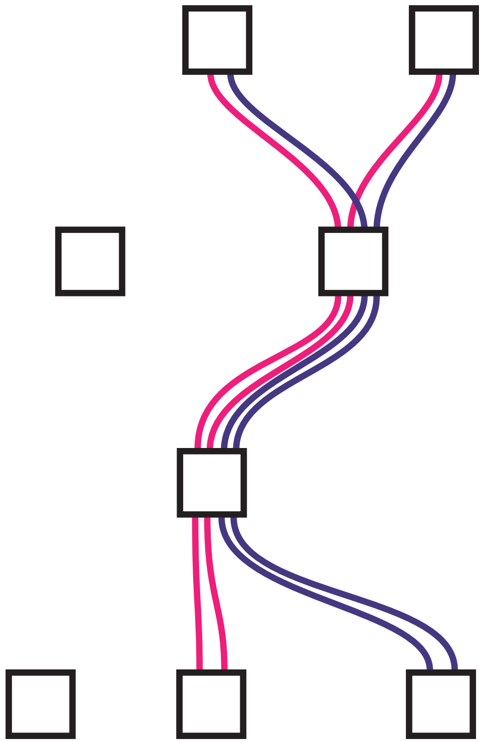
$$W_p = W_c W_b W_a$$

$$g_p = g_4 g_c g_3 g_b g_2 g_a g_1$$

$\bar{t}(p,e)$: target path of e

$\bar{s}(p,e)$: source path of e

Gradient descent



$$\tau \frac{d}{dt} W_e = \underbrace{\sum_{p \in \mathcal{P}(e)}}_{\mathcal{P}(e)\text{: All paths through } e} W^T_{\bar{t}(p,e)} \mathcal{E}(p) W^T_{\bar{s}(p,e)}$$

$\mathcal{P}(e)$: All paths through e

$$\mathcal{E}(p) = \Sigma^{yx}(p) - \underbrace{\sum_{j \in \mathcal{T}(p)}}_{\mathcal{T}(e)\text{: All paths terminating at same node as } p} \mathrm{W_j} \Sigma^{x}(j,p)$$

$\mathcal{T}(e)$: All paths terminating at same node as p

Correlation matrices

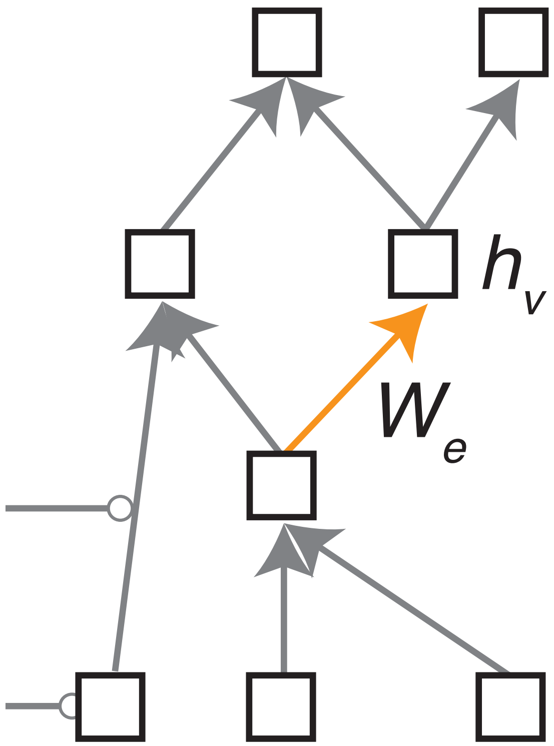
- Dynamics driven only by statistics:

$$\Sigma^{yx}(p) = \left\langle g_p y_{t(p)} x_{s(p)}^T \right\rangle_{y,x,g}$$

$$\Sigma^{x}(j,p) = \left\langle g_j x_{s(j)} x_{s(p)}^T g_p \right\rangle_{y,x,g}$$

- One correlation matrix per path

Intuition

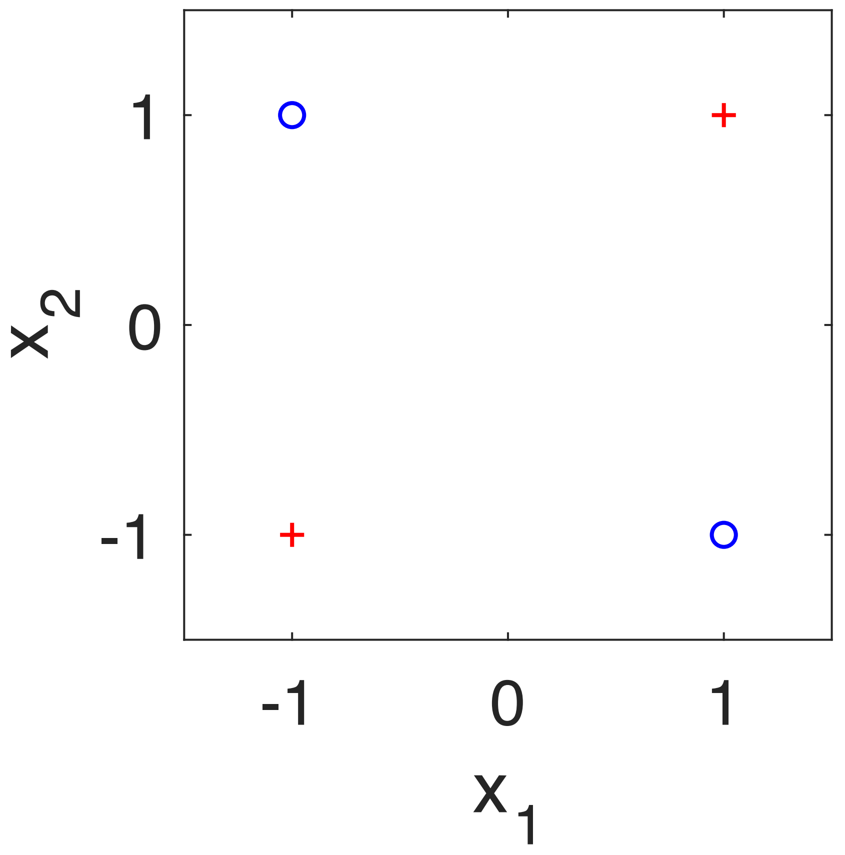


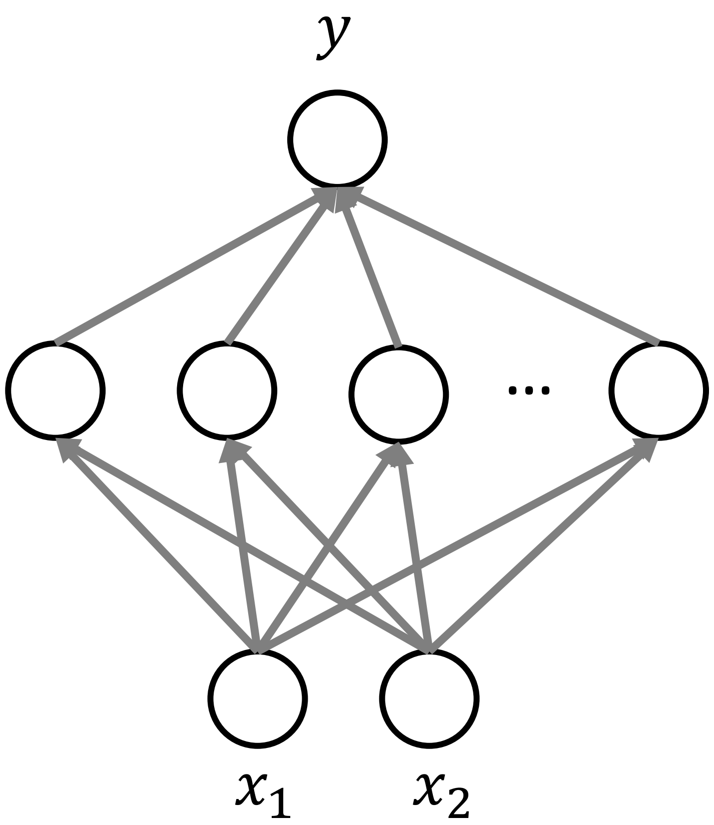
Each pathway behaves like a deep linear network

Gating controls the *effective dataset* for each pathway

All paths through an edge sum to determine dynamics

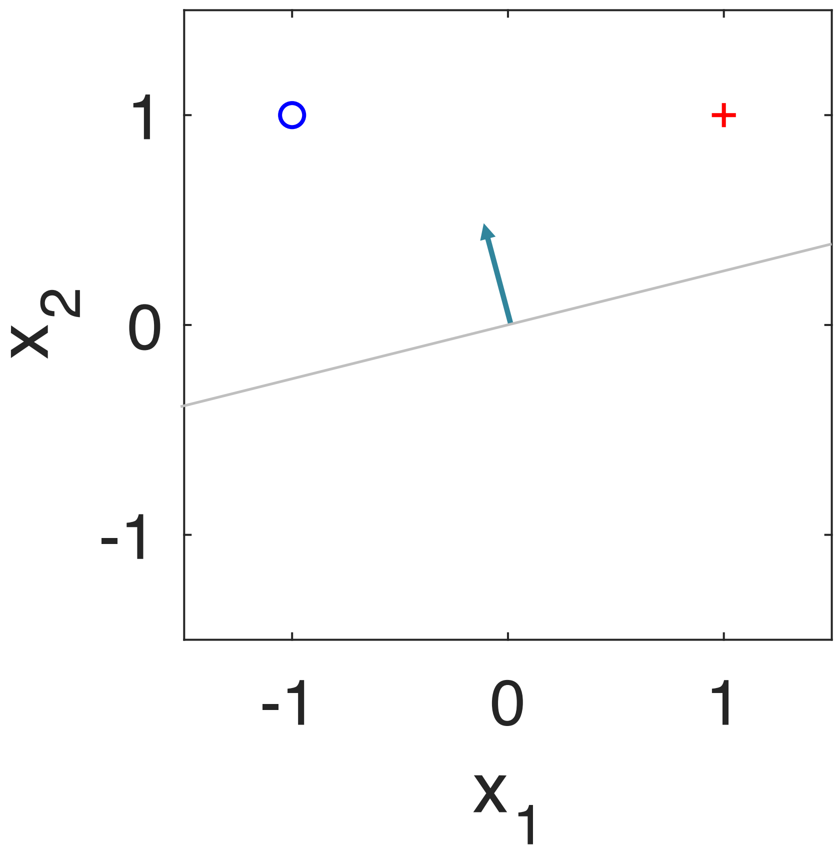
The XoR problem

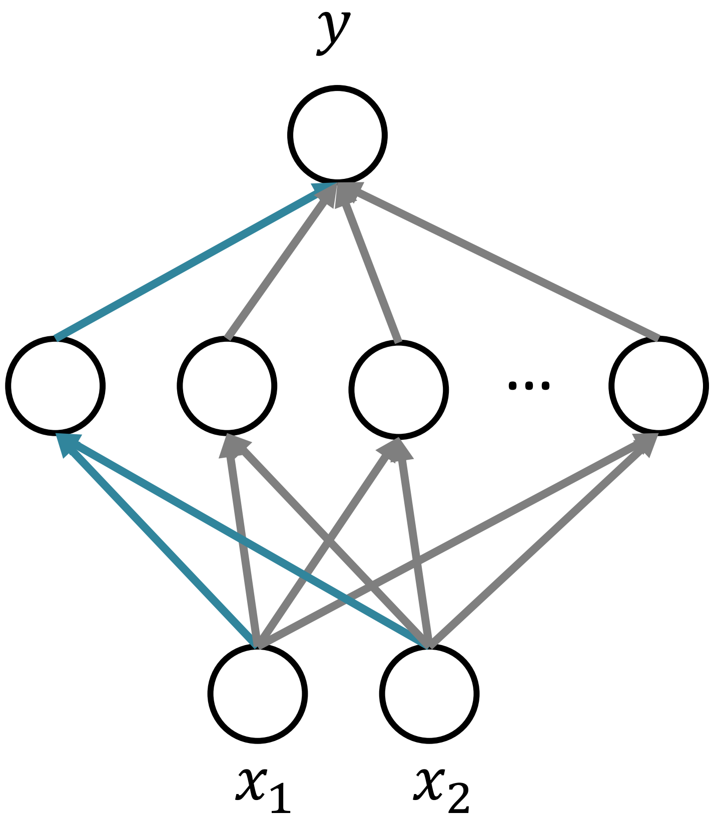




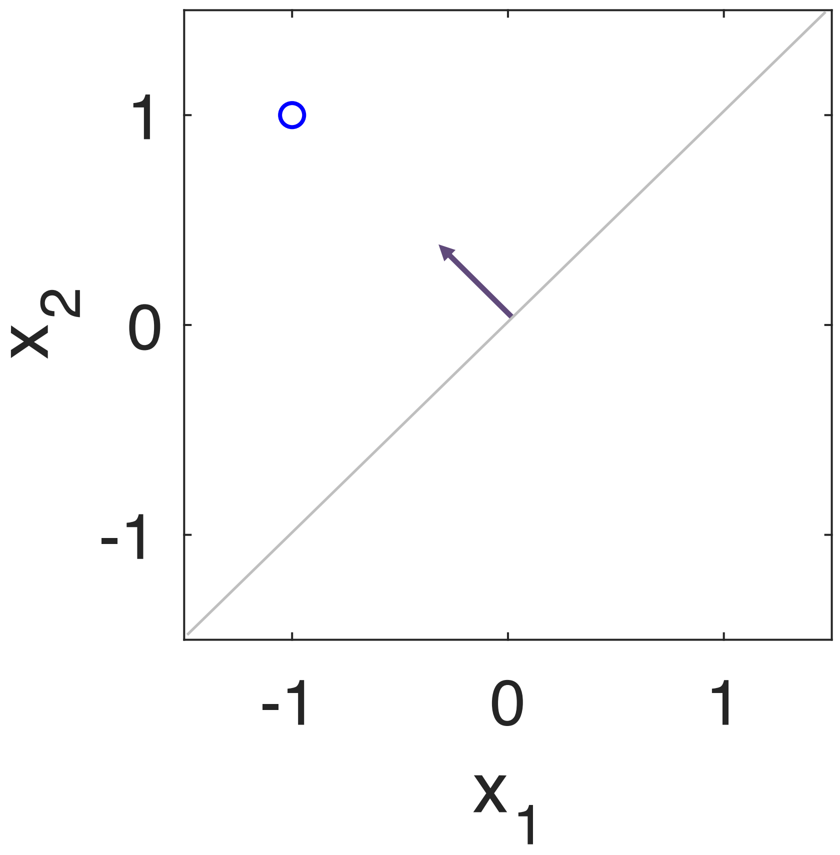
Minsky & Papert, 1969; Rumelhart, Hinton & Williams, 1986

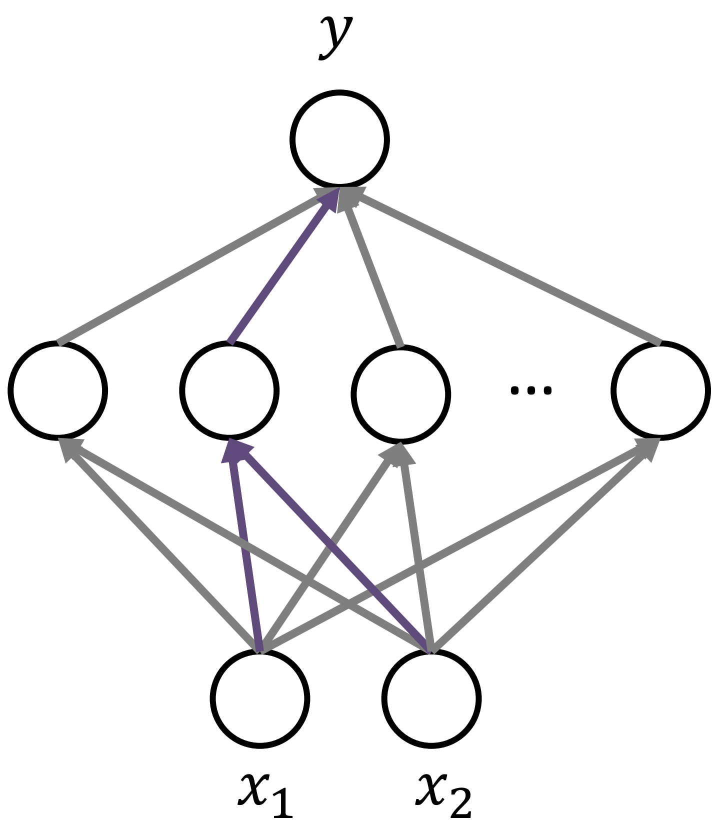
Gated dynamics



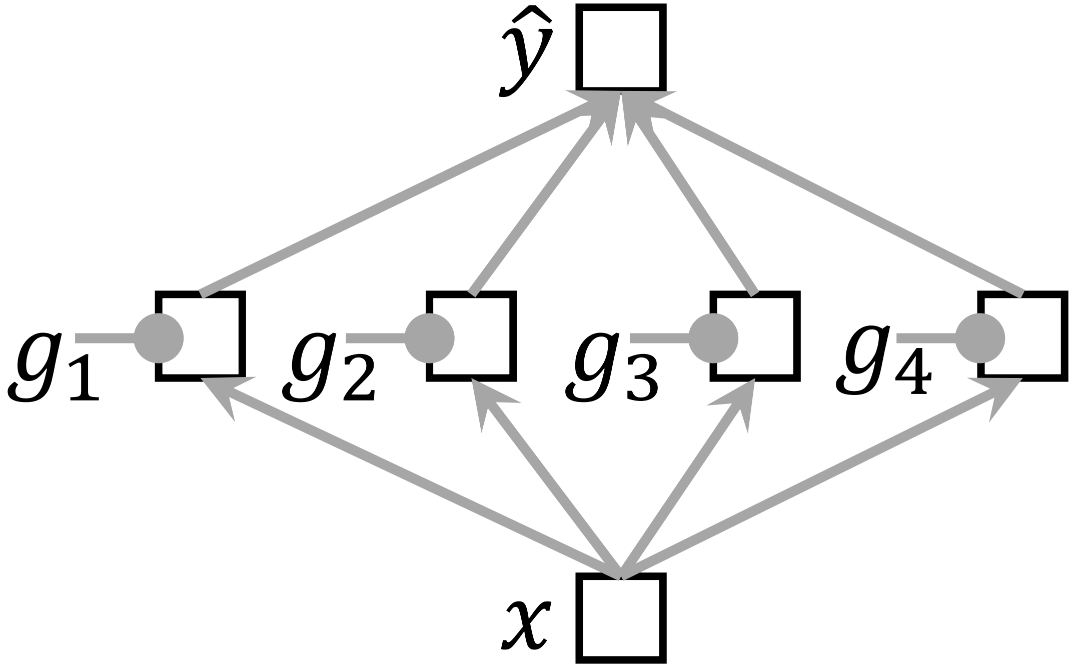


Gated dynamics



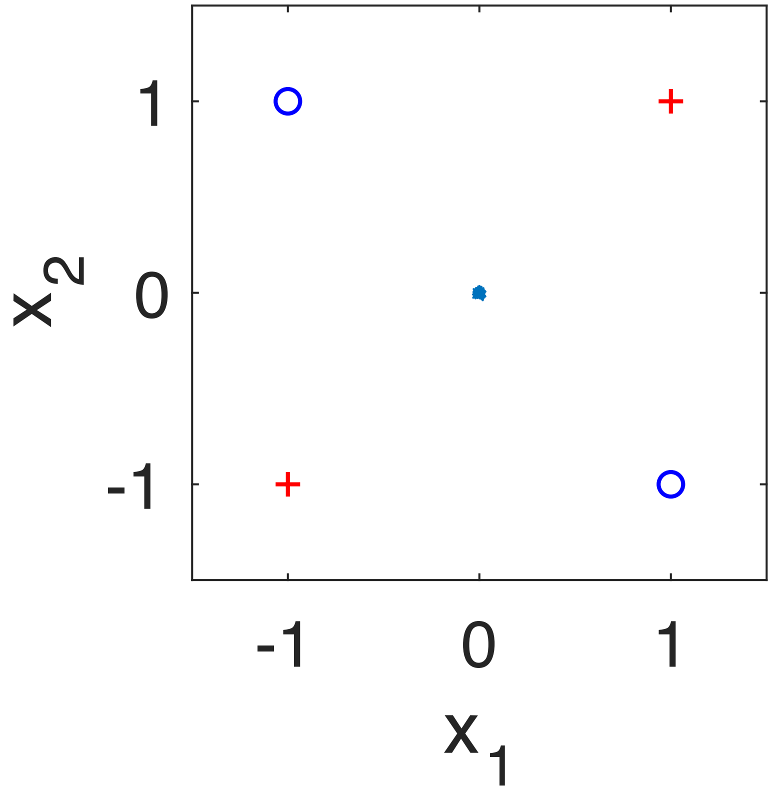


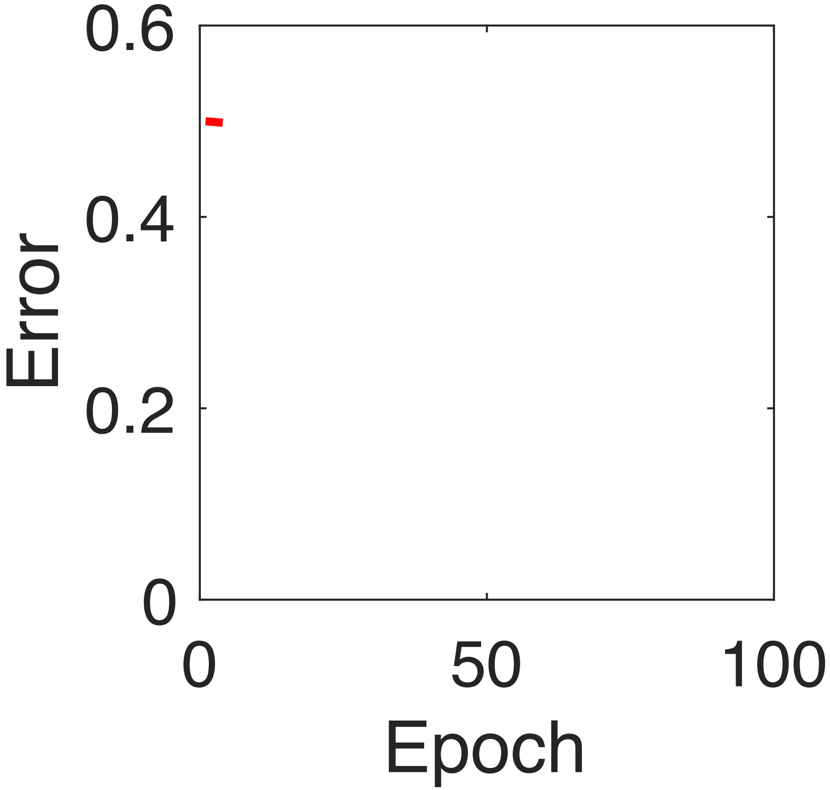
Gated DLN on XoR



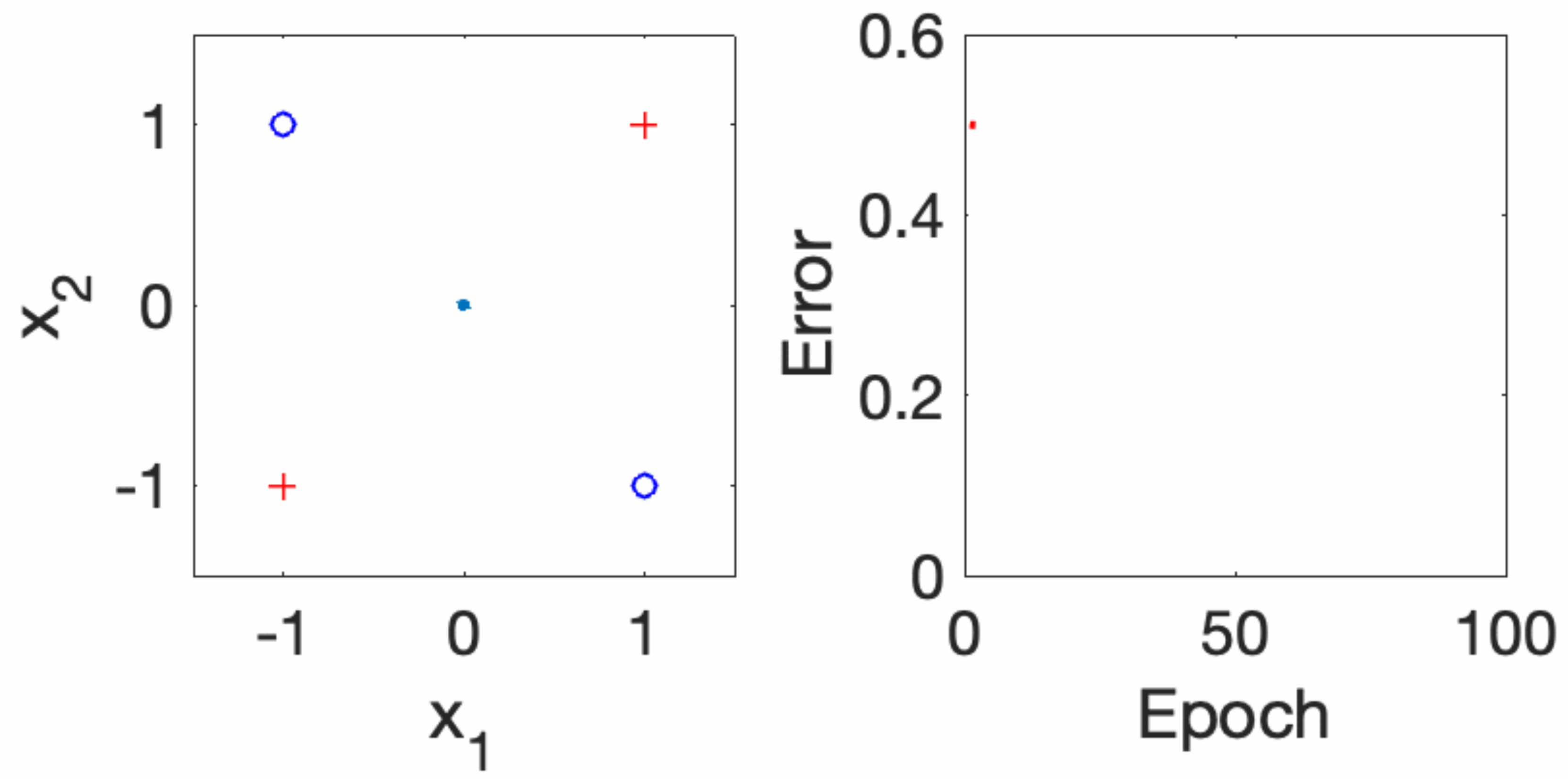
$$g_i = \begin{cases} 1 \text{ on example } i \\ 0 \text{ otherwise} \end{cases}$$

XoR Dynamics

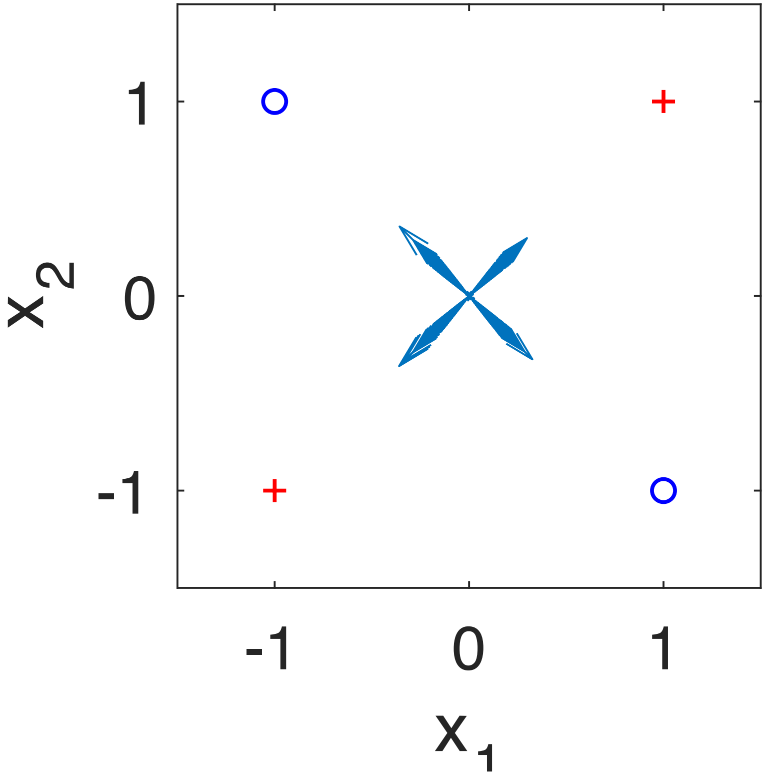


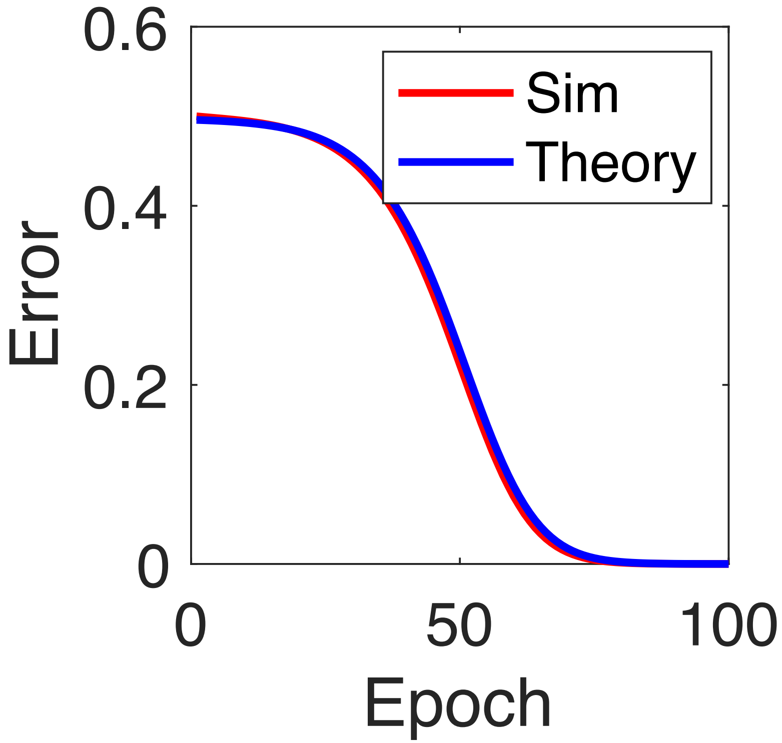


XoR Dynamics



XoR Dynamics





Reduction and (occasionally) exact solutions

"Decoupled" initialization: $$W_e(t) = R_{t(e)} B_e(t) R_{s(e)}^T \quad \forall e$$

Mutually diagonalizable correlations:
$$\begin{aligned} \Sigma^{yx}(p) &= U_{t(p)} S(p) V_{s(p)}^T \\ \Sigma^{x}(j,p) &= V_{s(j)} D(j,p) V_{s(p)}^T \end{aligned}$$

Reduction: $$\tau \frac{d}{dt} B_e = \sum_{p \in \mathcal{P}(e)} B_{p \setminus e} \left[S(p) - \sum_{j \in \mathcal{T}(t(p))} B_j D(j,p) \right]$$

Assumptions & caveats

- Reduction exact for GDLNs

- Also exact for ReLU networks under the assumptions:
  - Gates on each example match the activity set
  - No neurons switch their activity set
  - Initial weights are decoupled

- Can approximate ReLU networks with small random weights, but not always

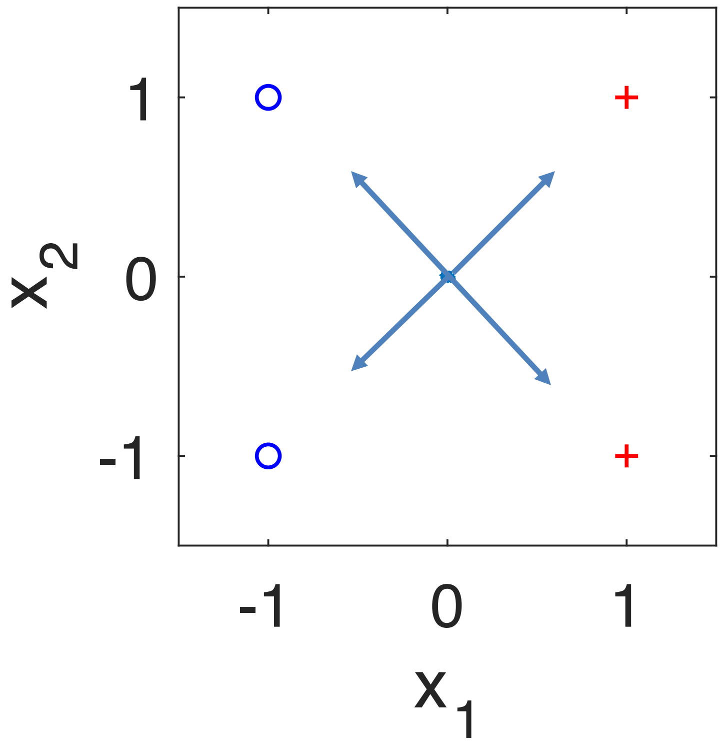
The neural race reduction

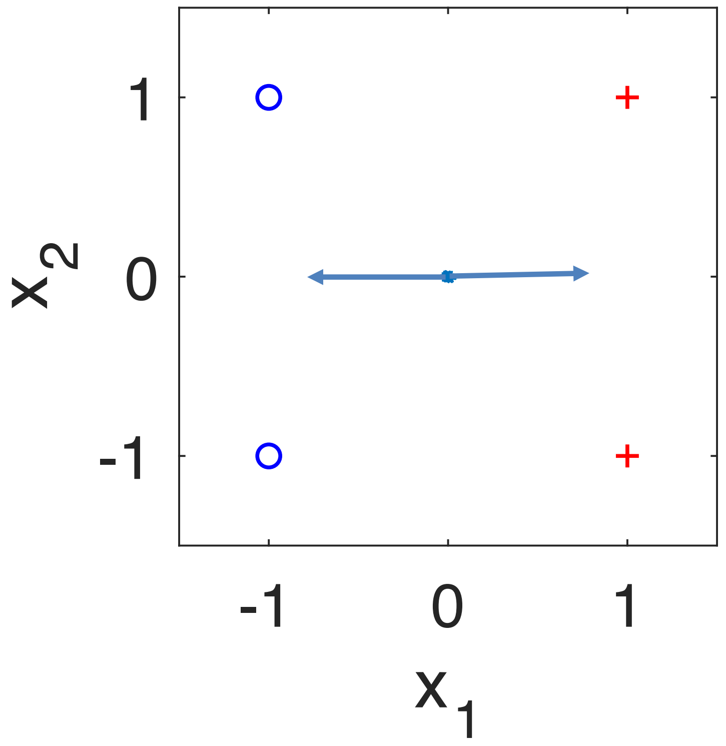
- In a large network with many pathways, these compete to reduce the global error

- A pathway's learning speed depends on:
  - Effective dataset (larger input-output correlation faster)
  - Pathway depth (deeper generally slower)
  - Initialization (larger/imbalanced generally faster)
  - Edge sharing (more pathways through edge generally faster)

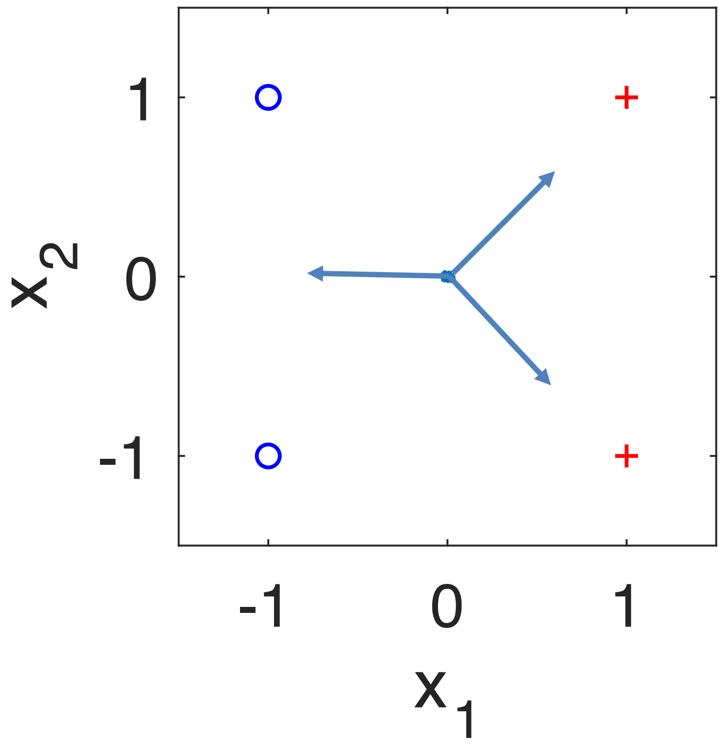
- The fastest pathways can dominate the solution

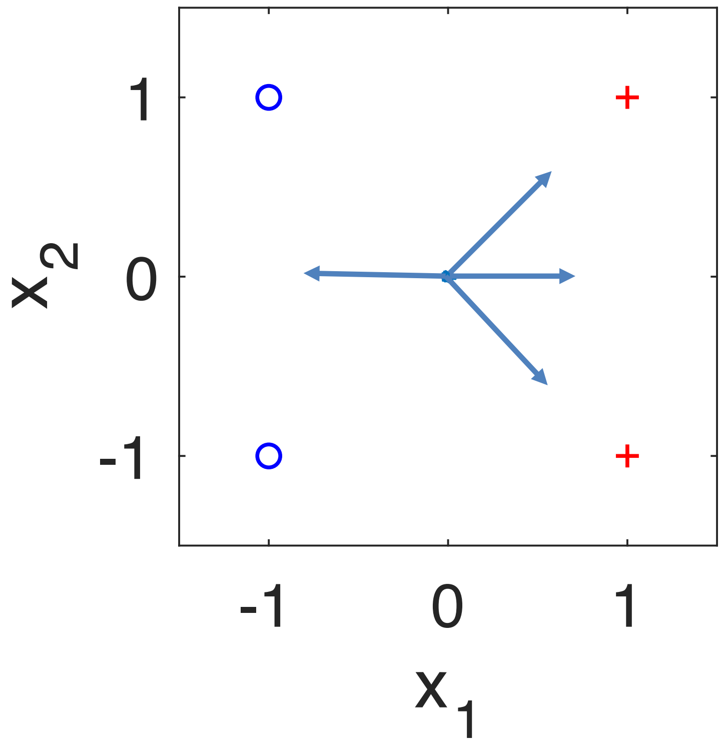
Which gating structures?





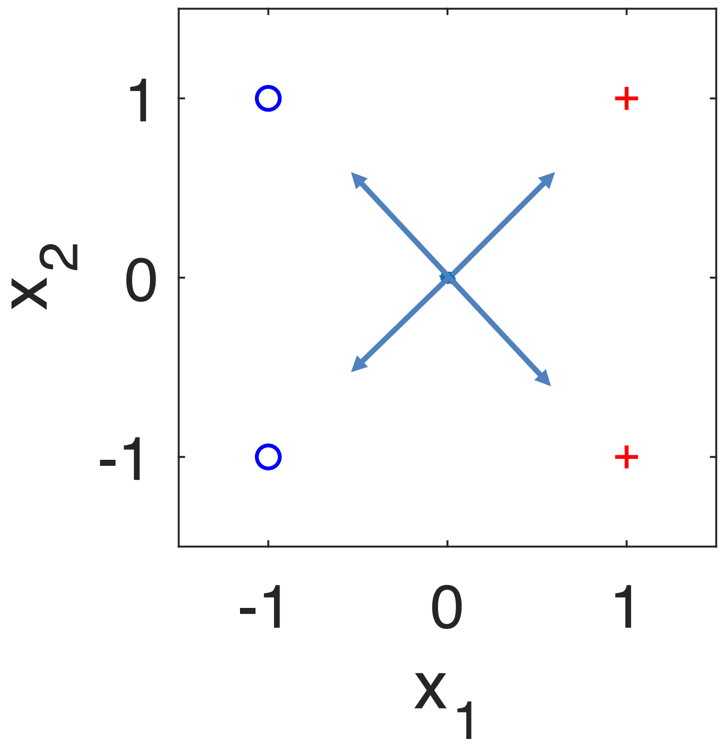
Which gating structures?

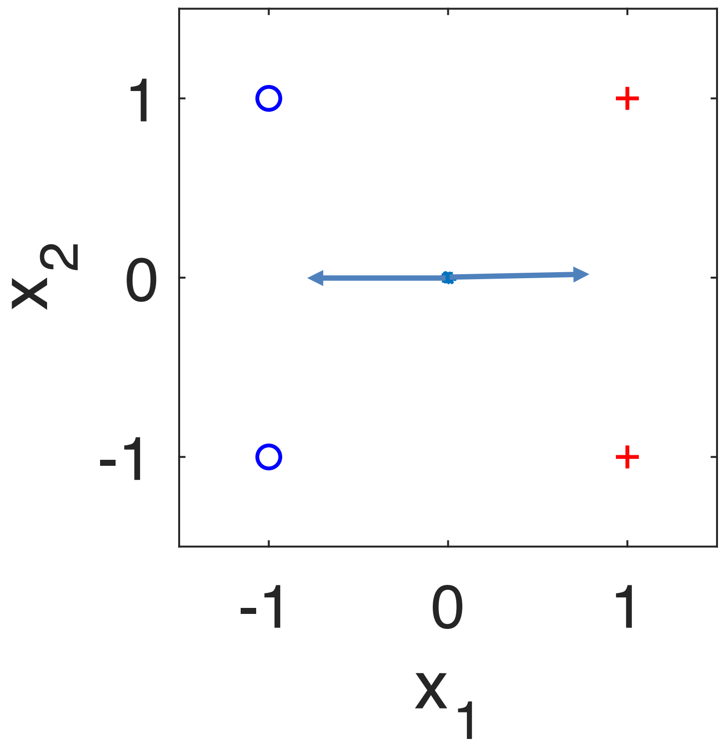




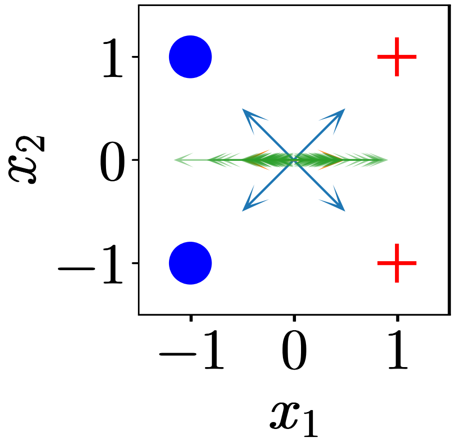
Neural Race Reduction

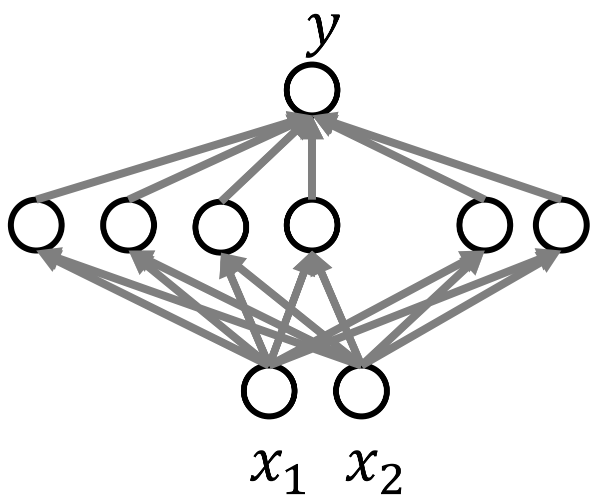
- Each gating scheme yields a distinct effective dataset and deep linear network trajectory
- The one which learns fastest dominates the solution

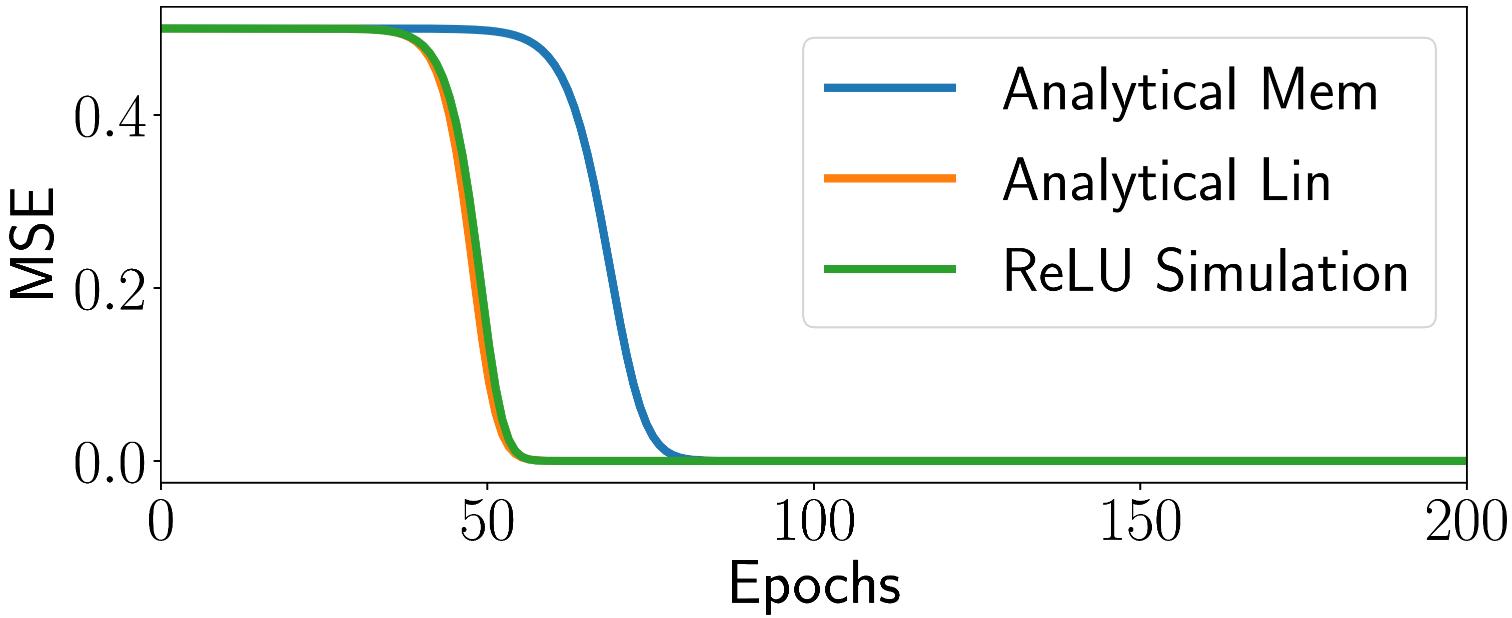




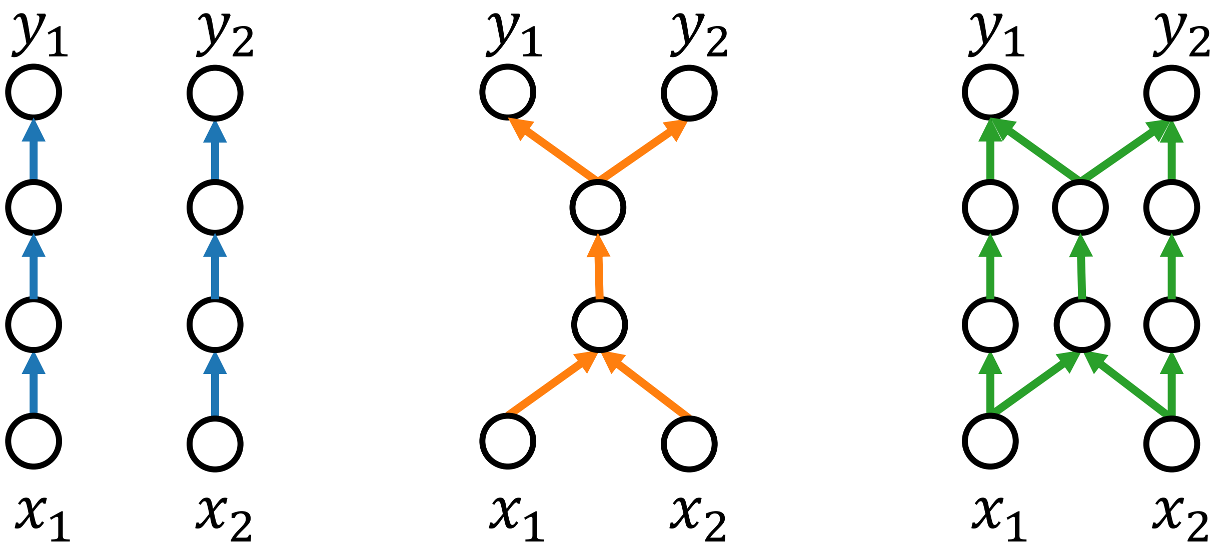
The neural race: stronger input-output correlations

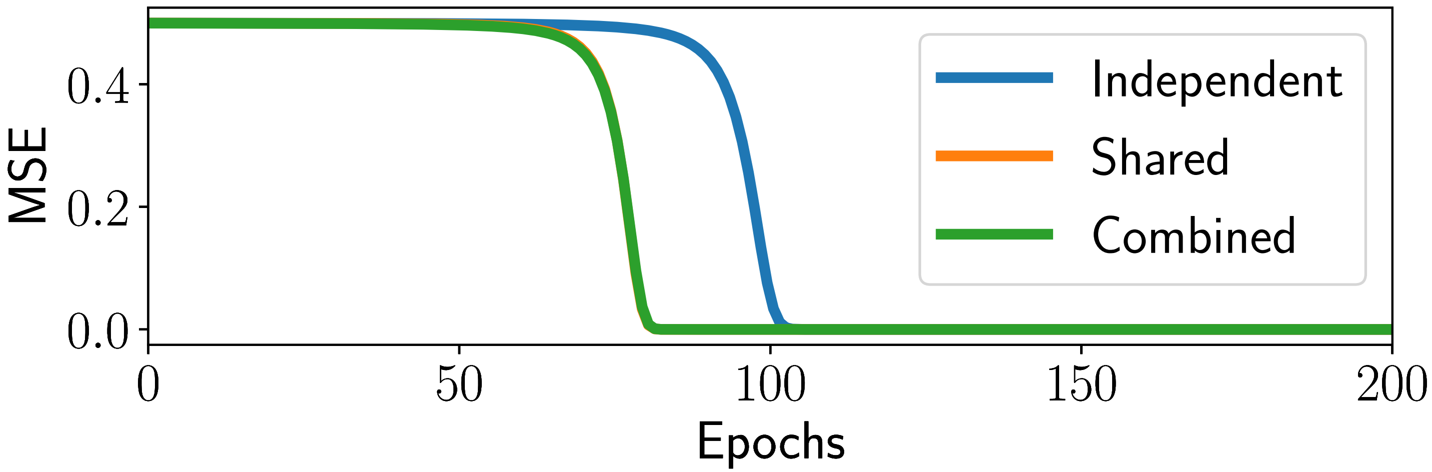




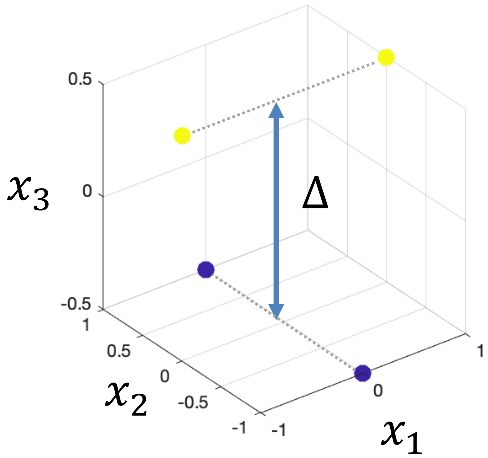


The neural race: edge sharing

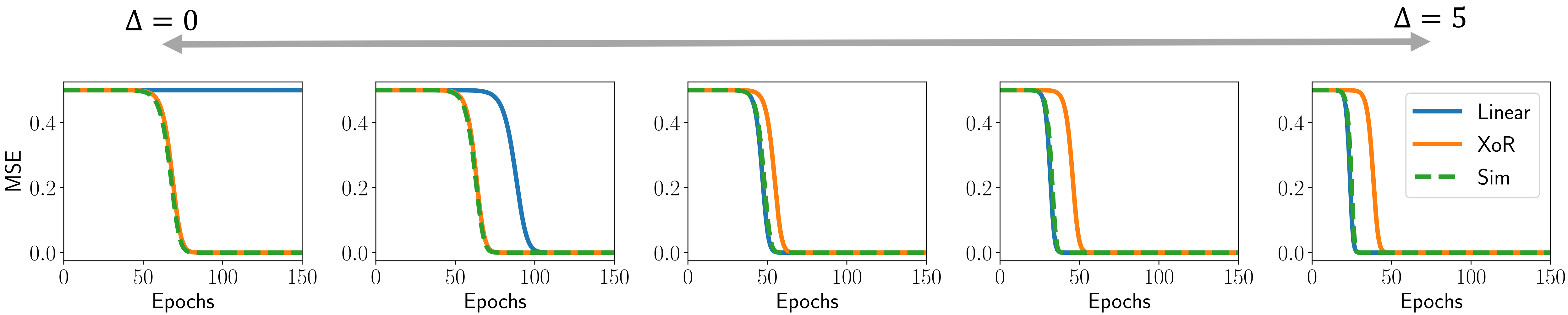




Example: transition to nonlinearity

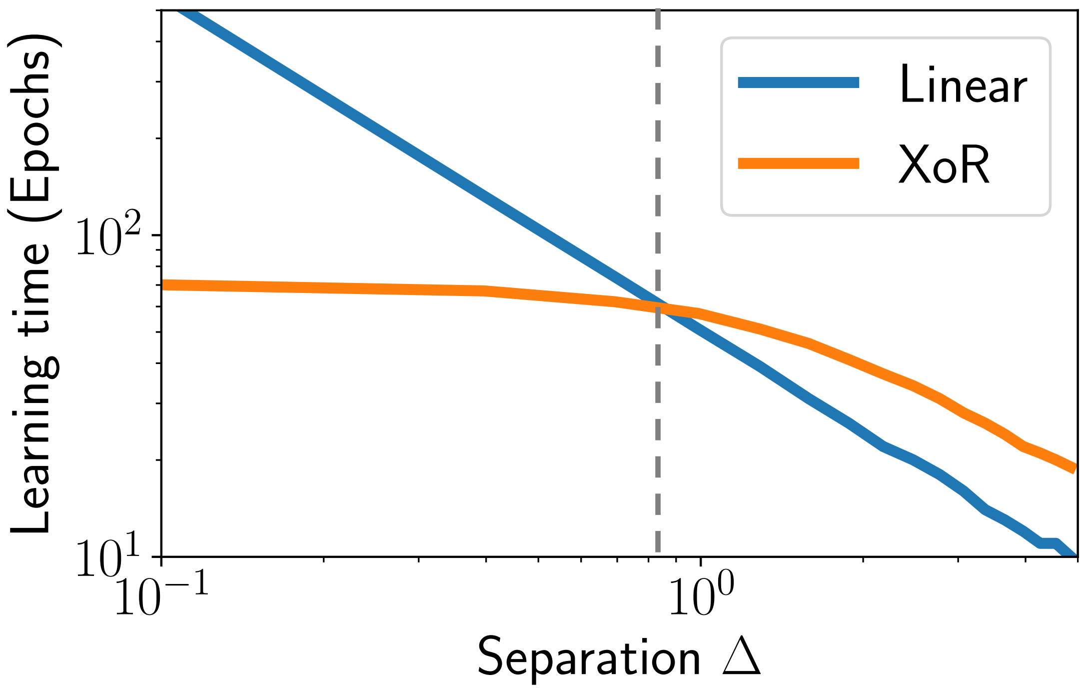


linearly separable with margin Δ for any $\Delta > 0$,
collapses to XoR at $\Delta = 0$



Example: transition to nonlinearity

$$\Delta_{\text{switch}} = \sqrt{2/3}$$

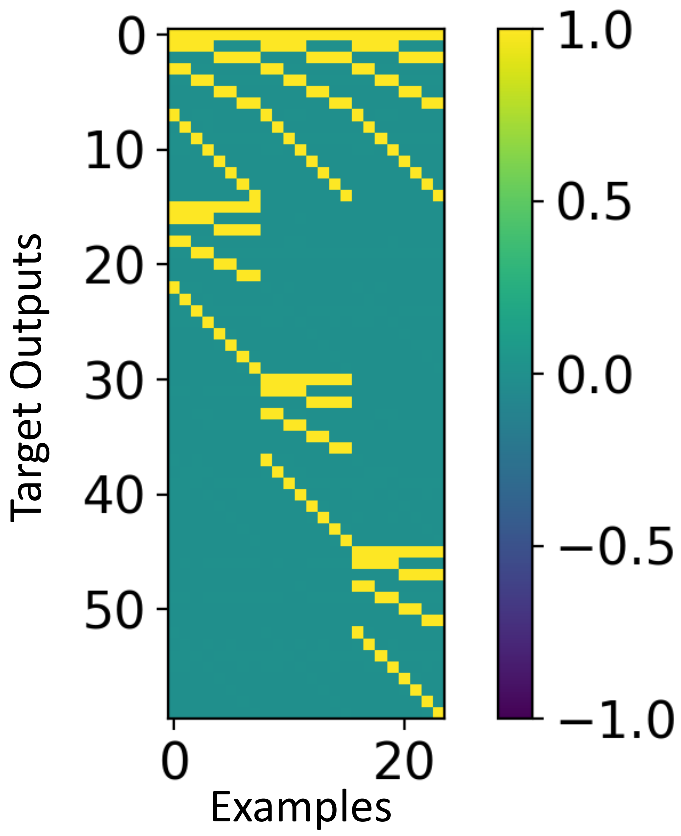


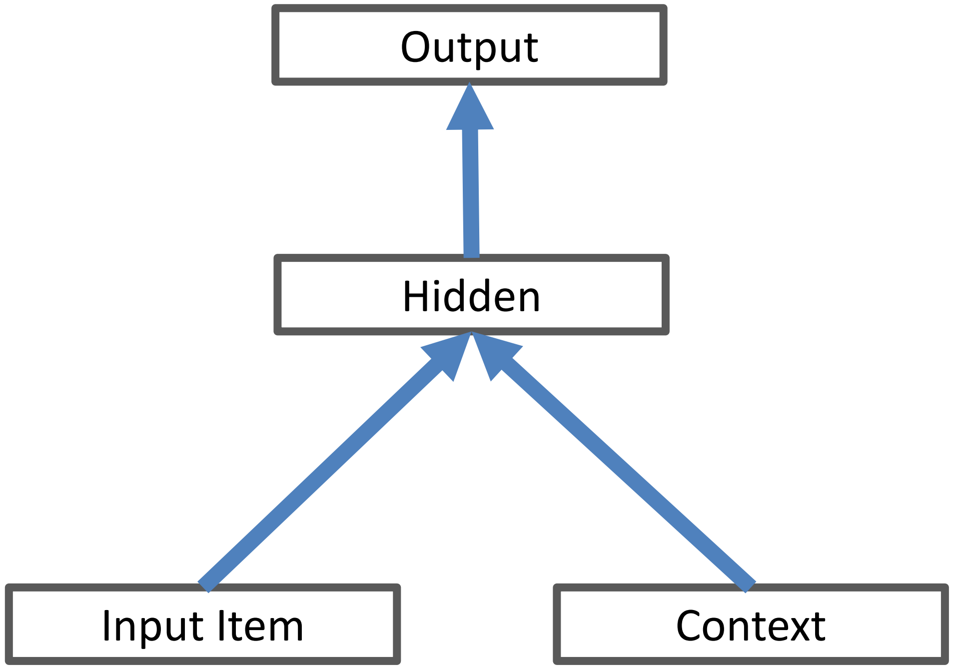
$$s_{lin} = \Delta/2$$

$$s_{XoR} = \frac{\sqrt{2 + \Delta^2}}{P}$$

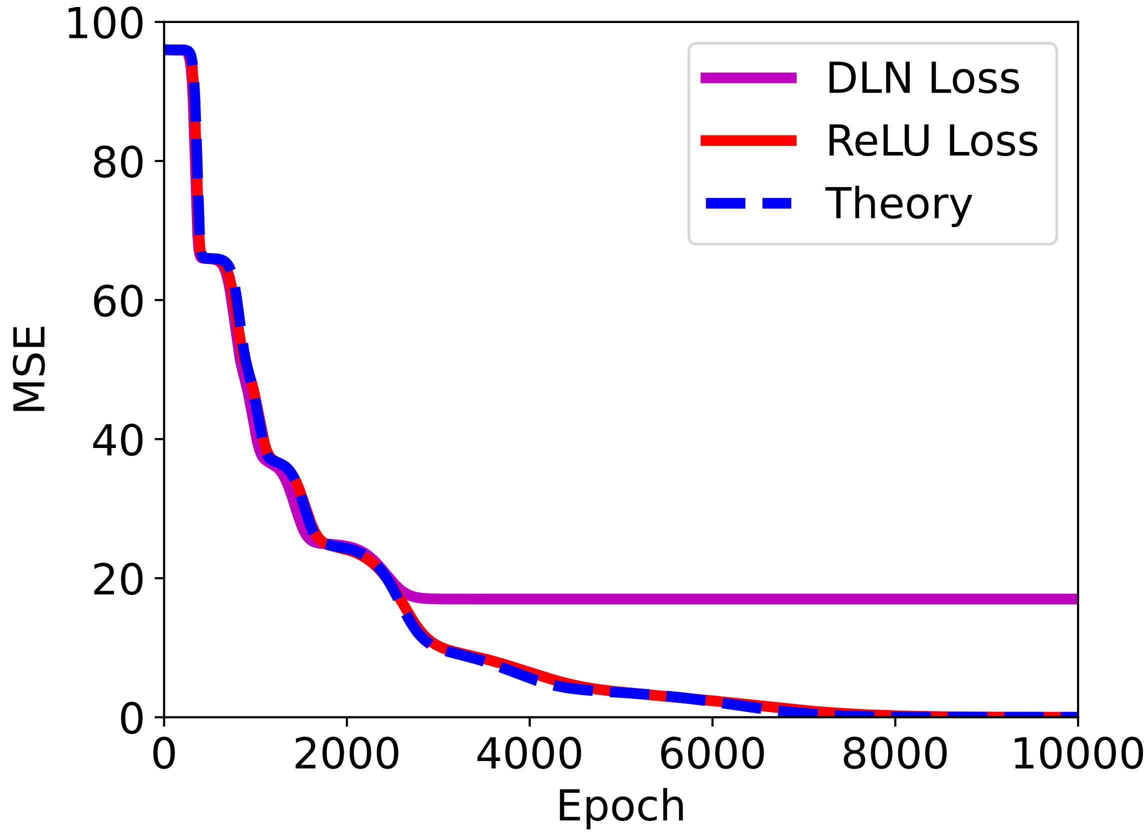
Nonlinear representations emerge before they are strictly necessary

Context-dependent Processing

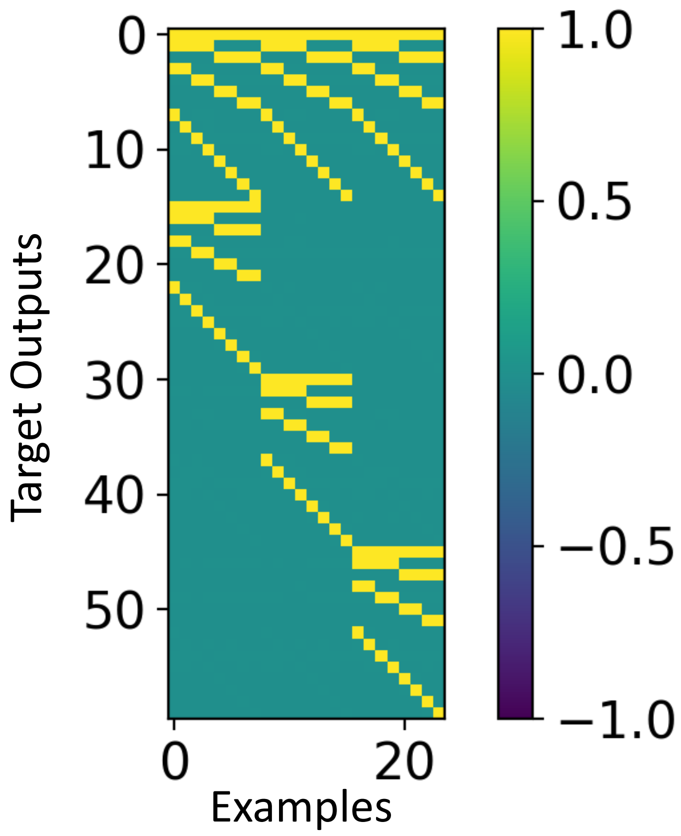


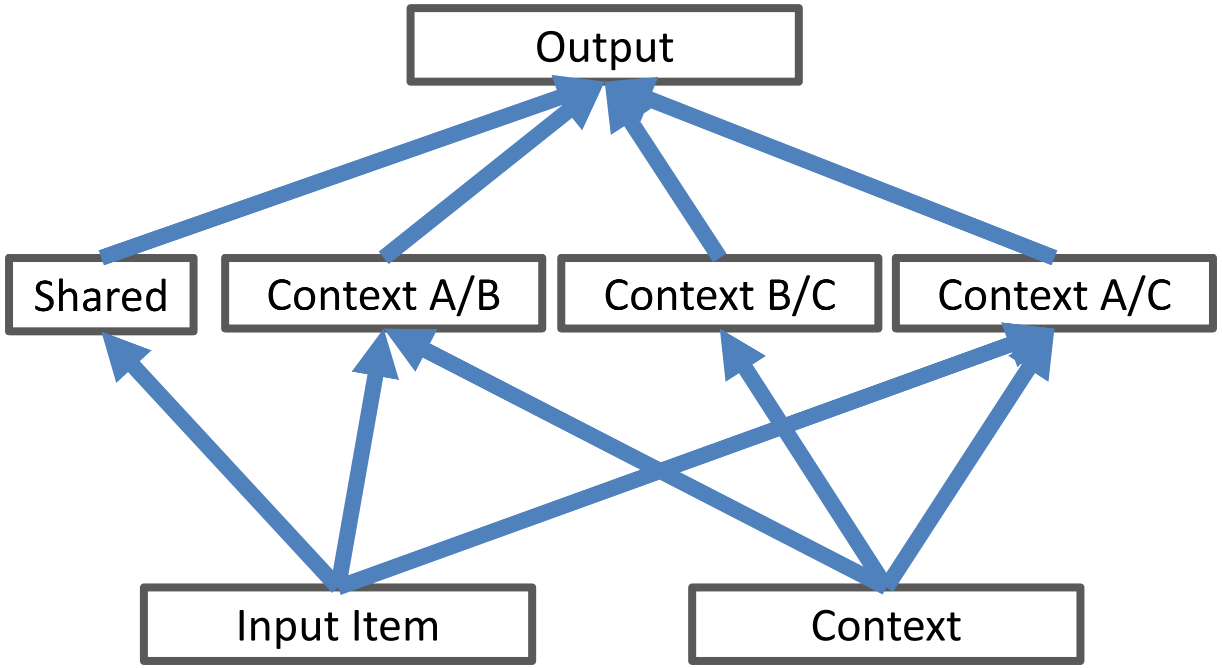


Context-dependent Processing

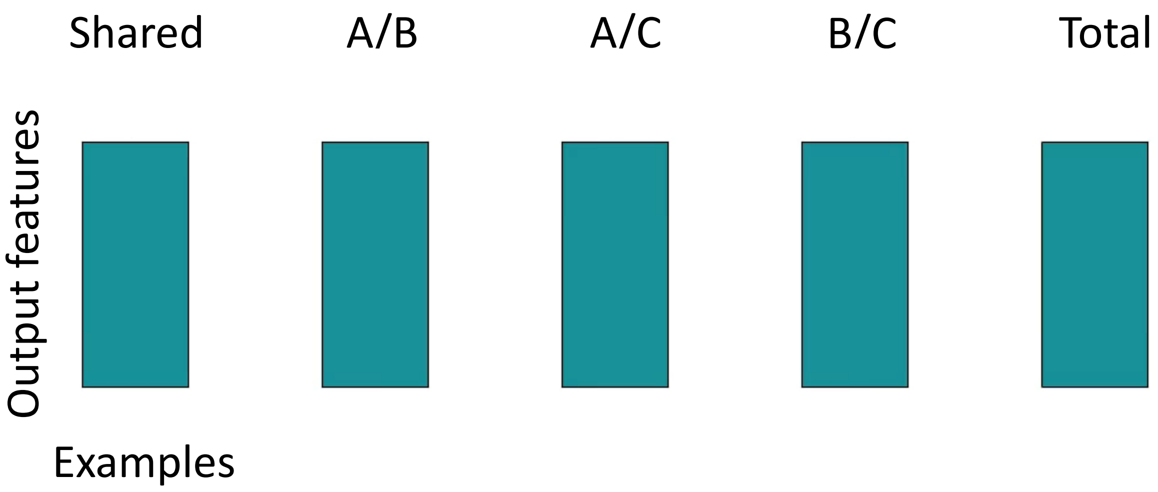


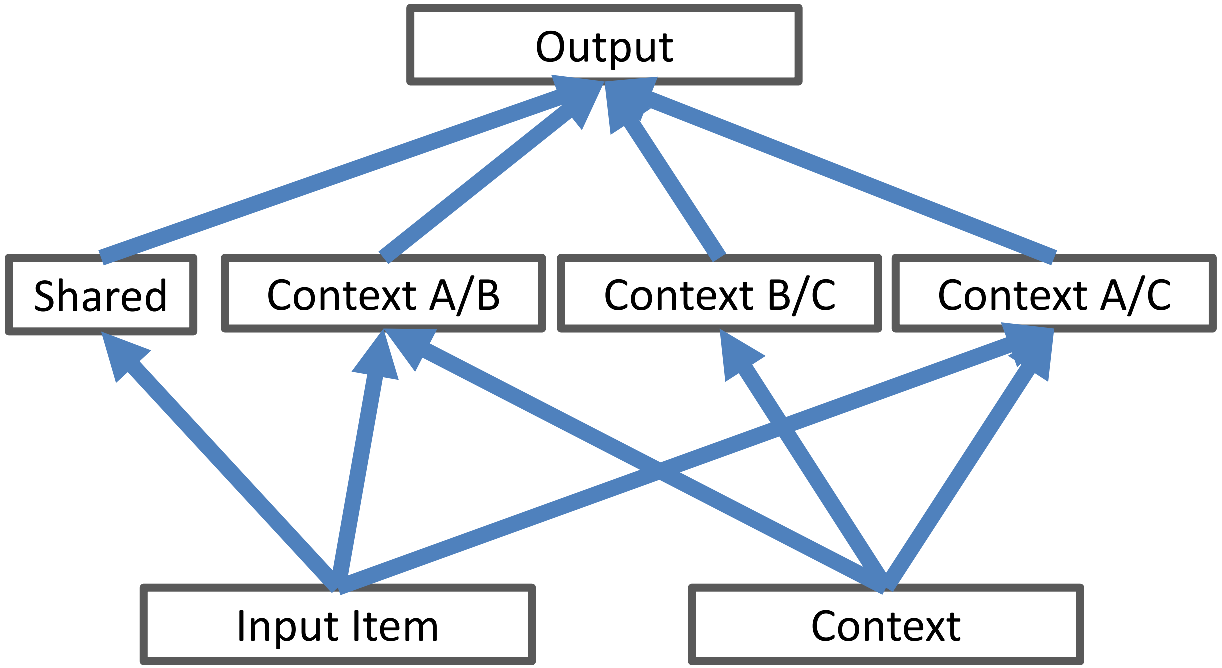
Context-dependent Processing



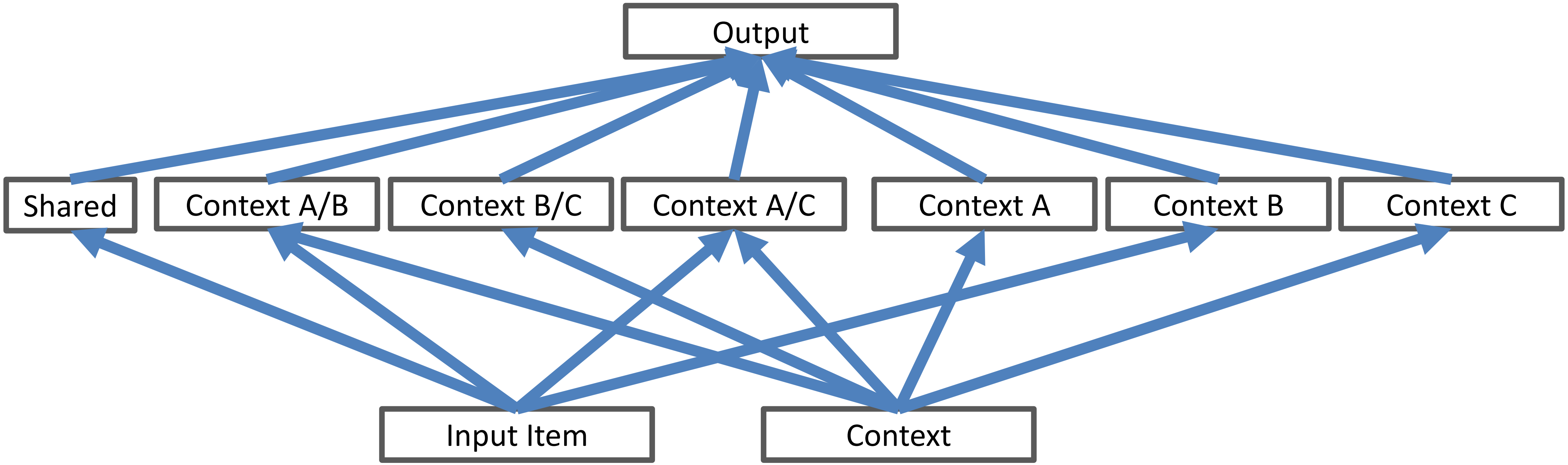


Context-dependent Processing

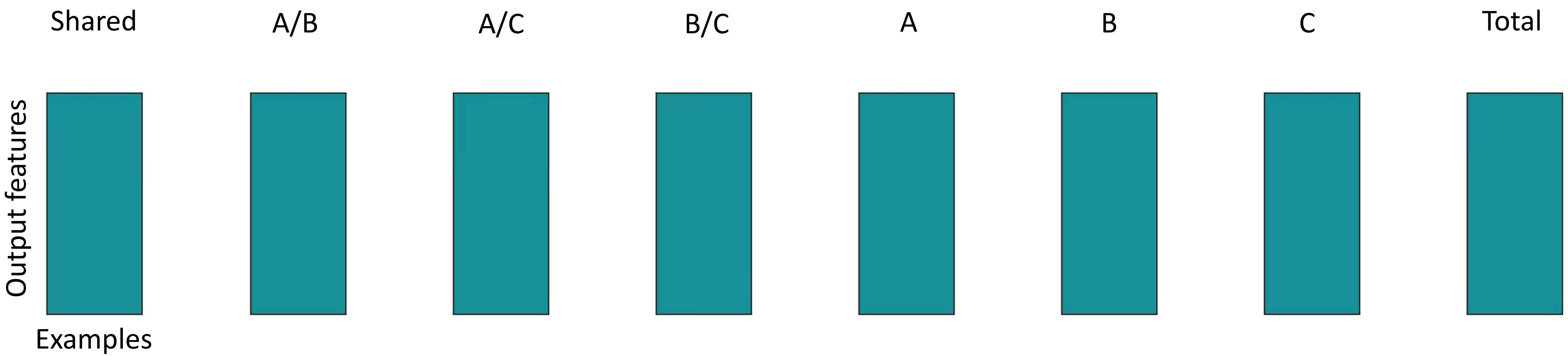




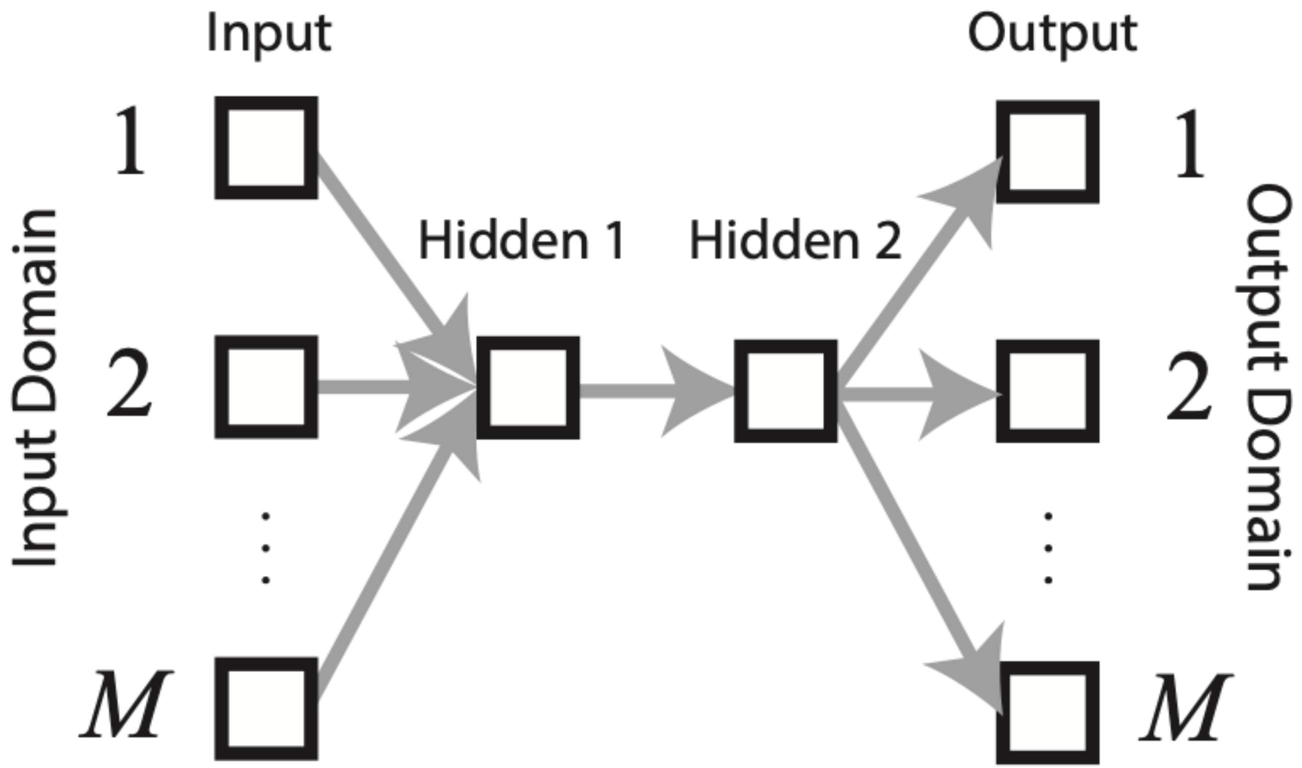
Context-dependent processing



Context-dependent processing



Example: Routing network

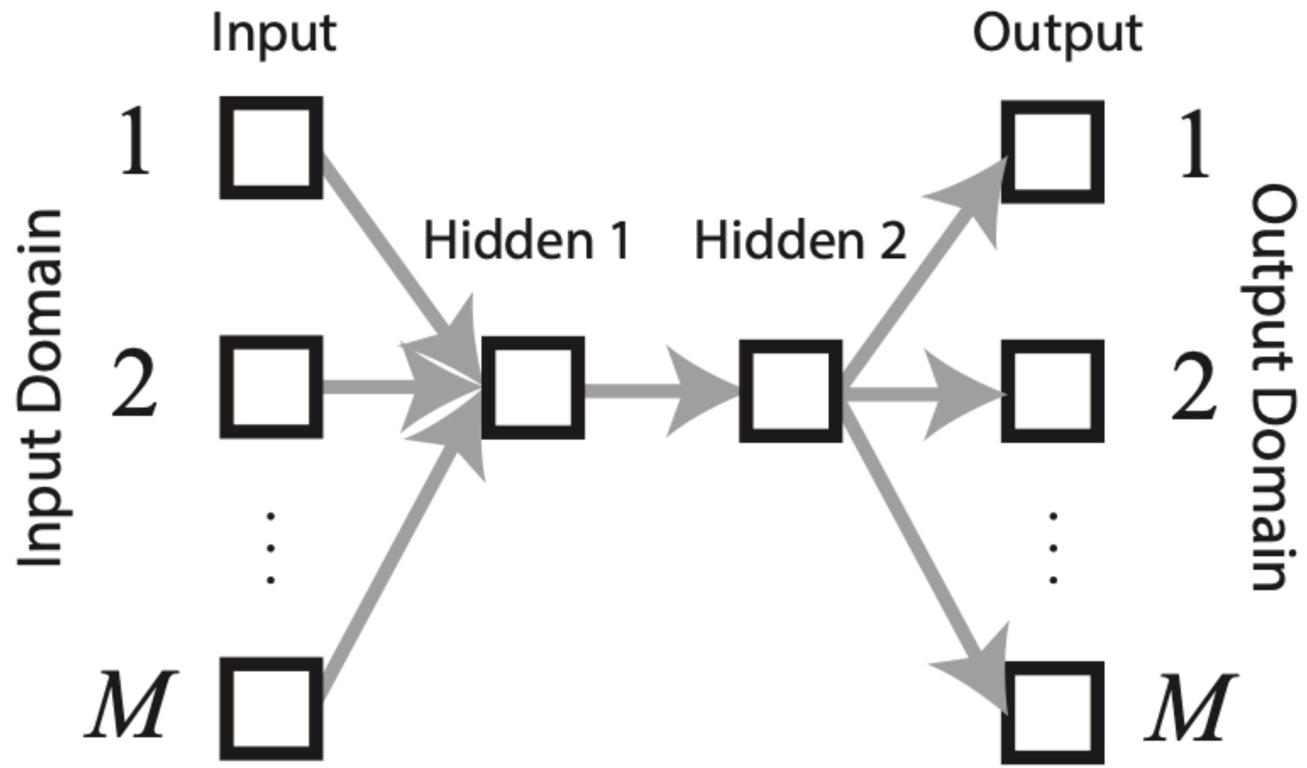


Ex: multilingual translation

French

German

Spanish



French

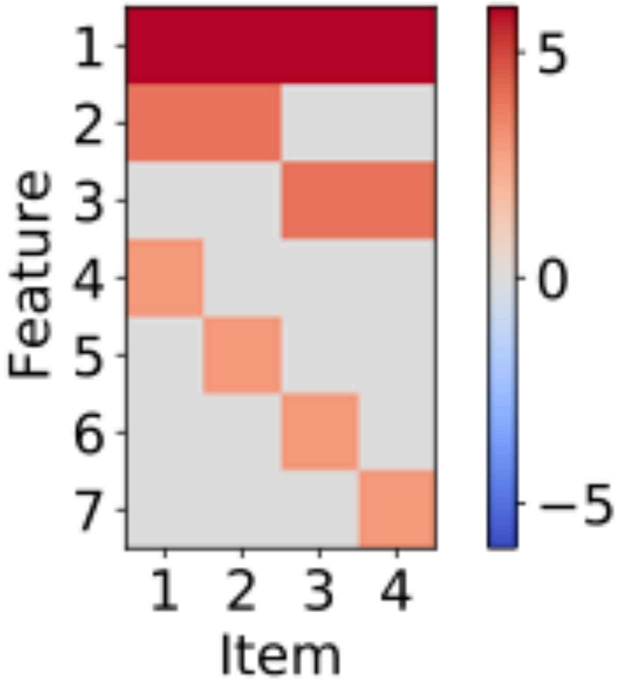
German

Spanish

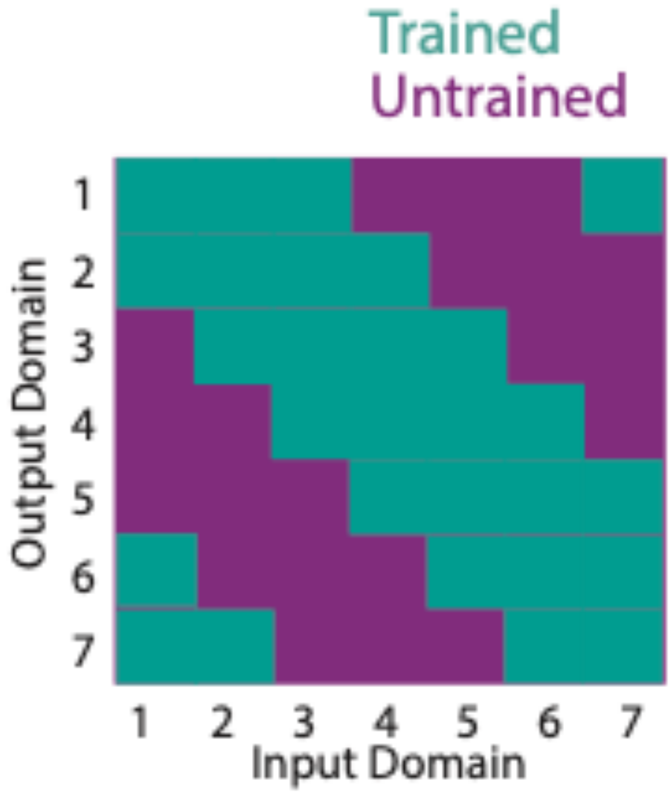
Each domain has distinctive inputs/outputs but similar underlying structural form

Dataset

Simple hierarchical dataset for each domain

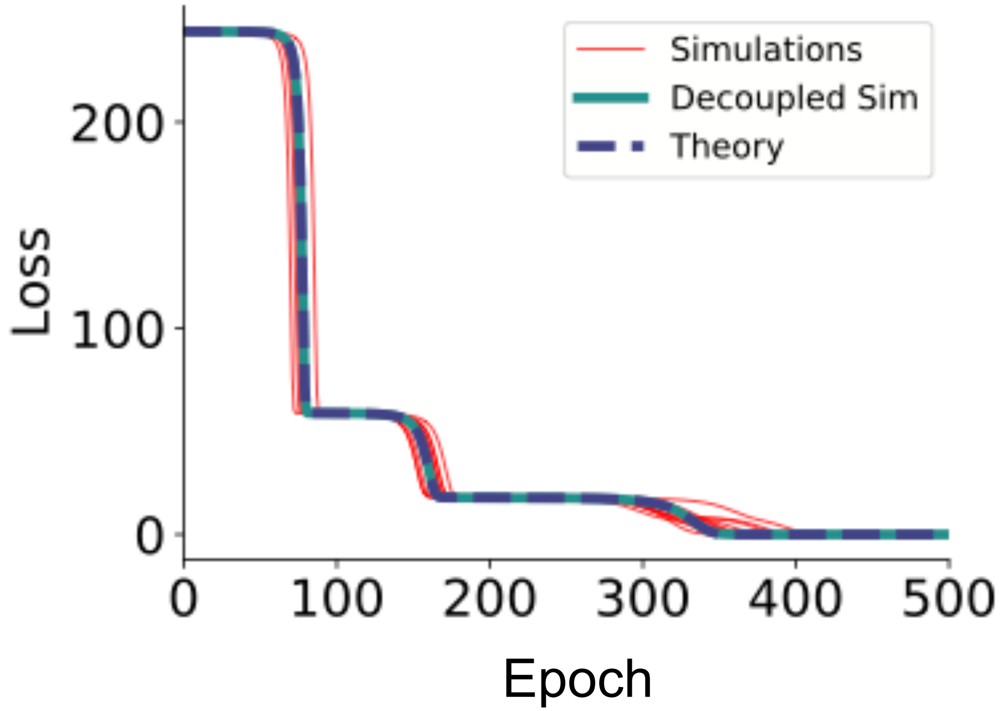


Subset of trained domain pairs

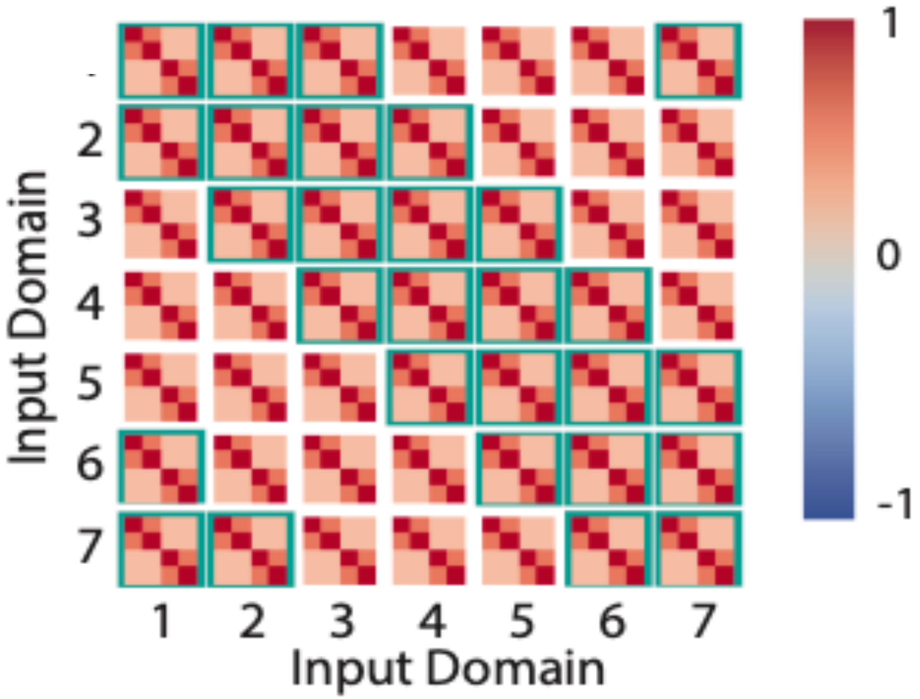


M: # domains
K: # trained output domains per input domain

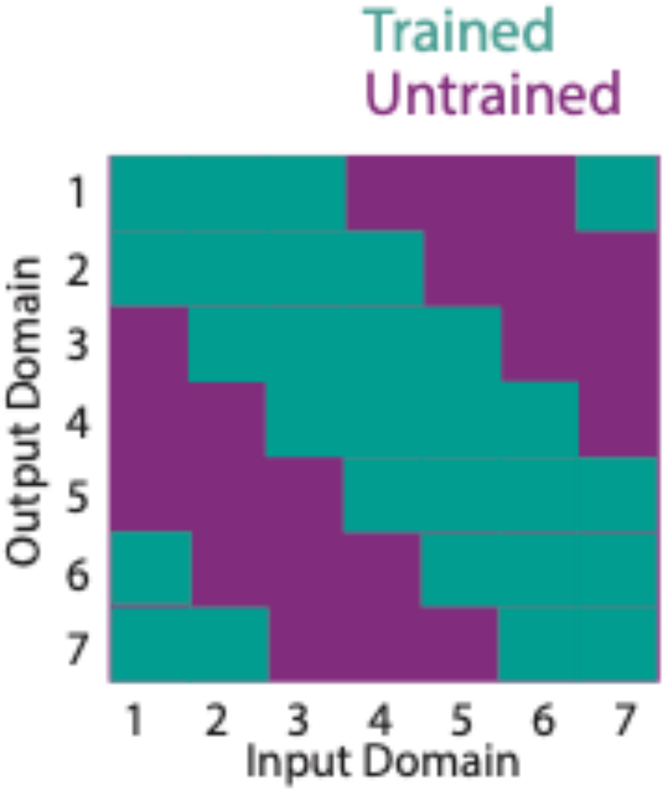
Dynamics of abstraction

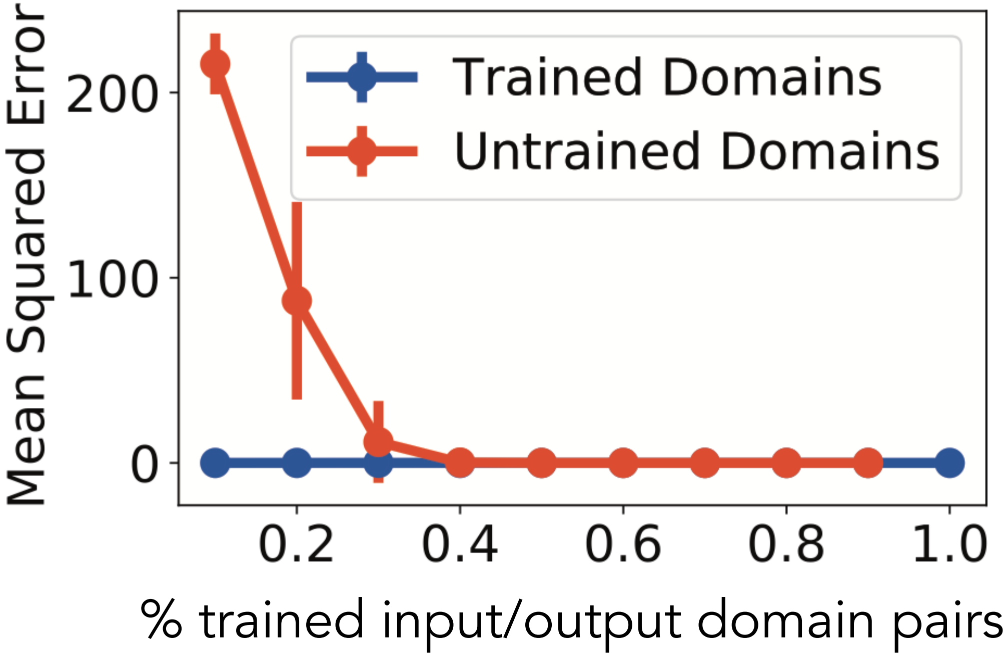


1st hidden layer RSA



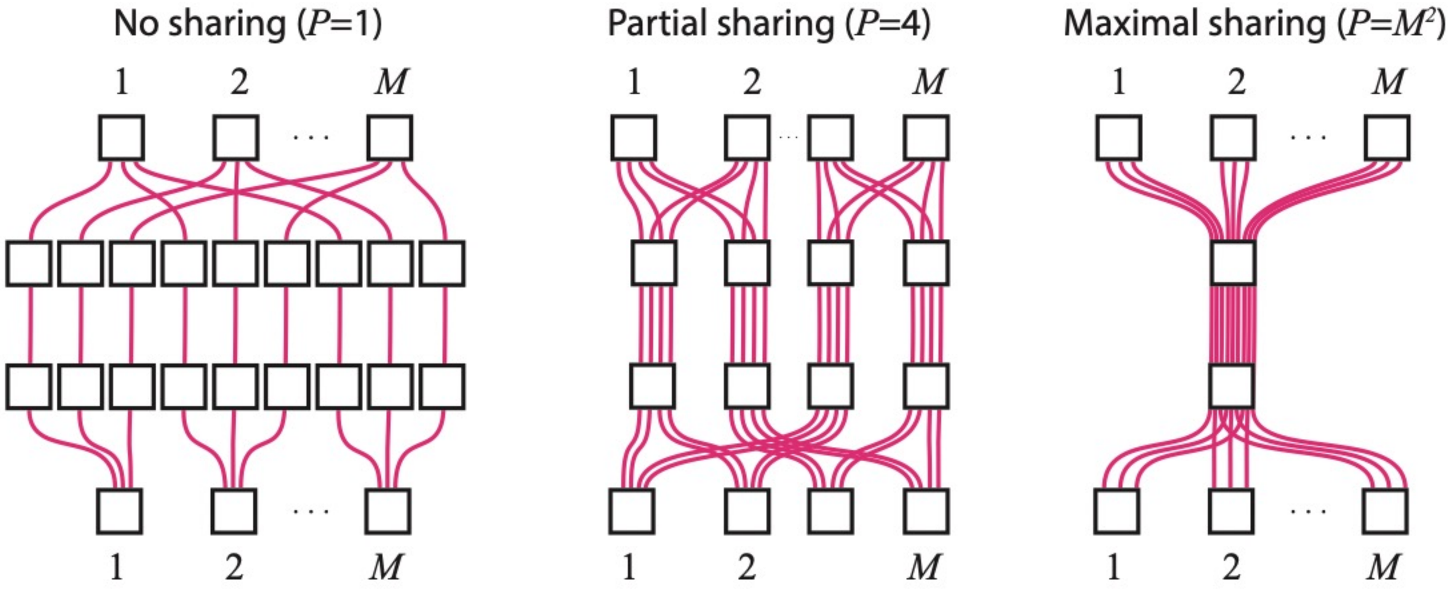
Systematic generalization

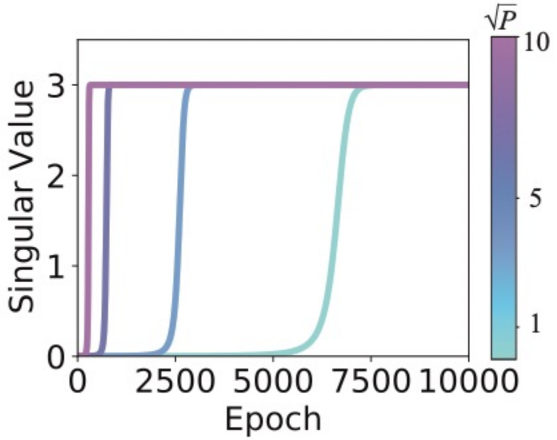


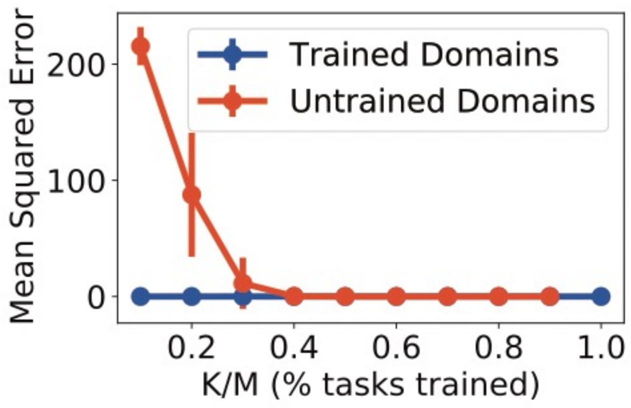


Saxe*, Sodhani*, & Lewallen, ICML 2022

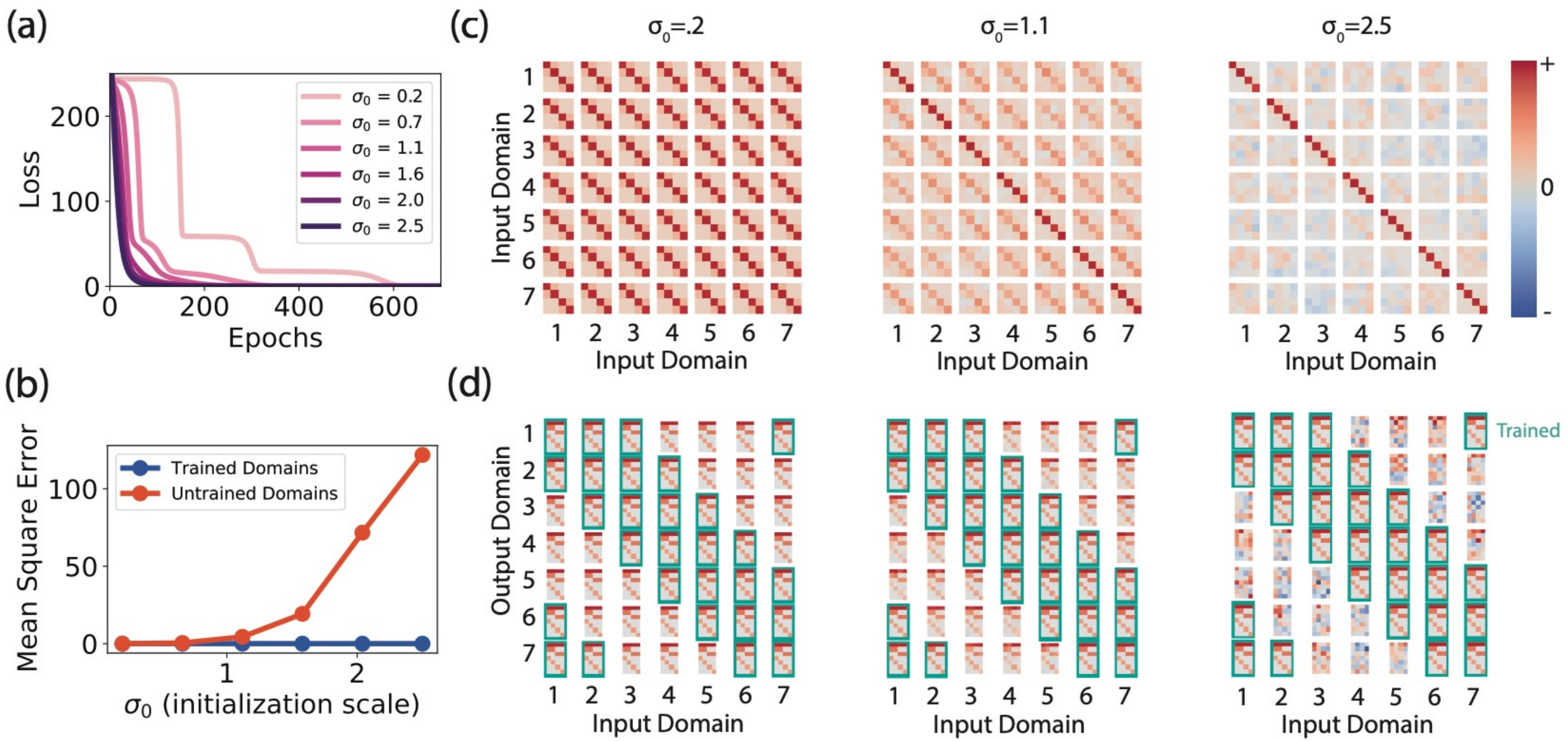
Race dynamics favor shared structure



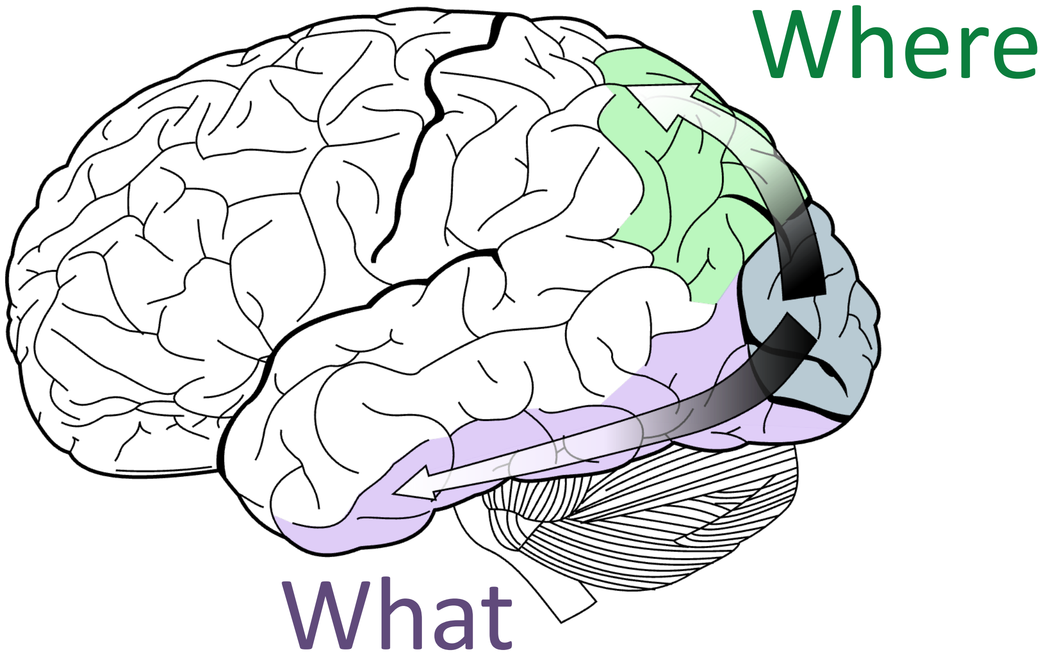


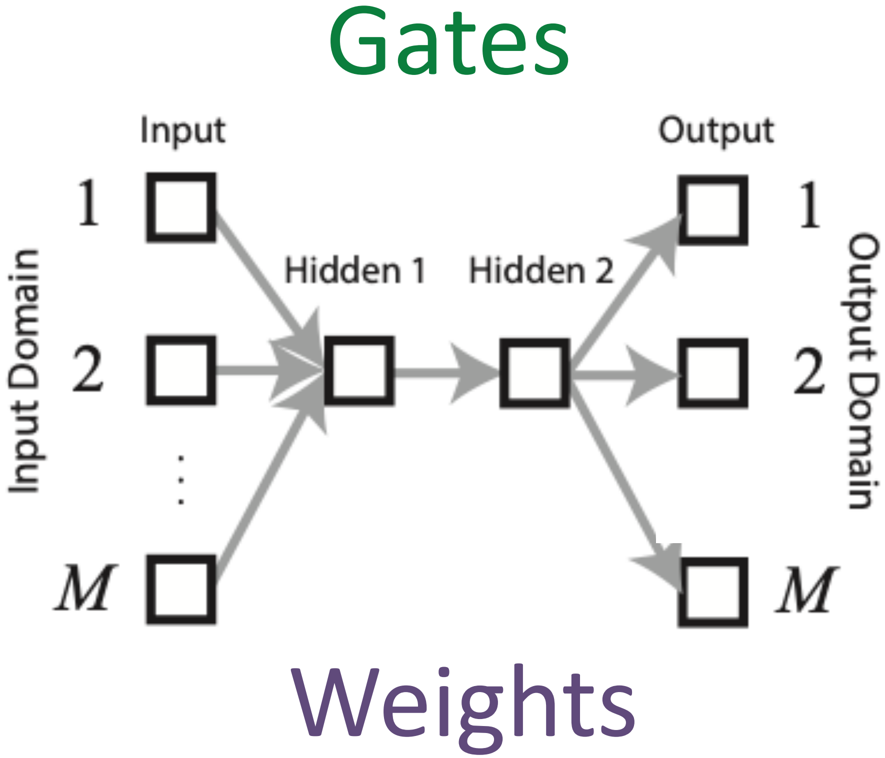


Initialization dependence: rich vs lazy learning



Factorization & principle of convergence





Selket, https://commons.wikimedia.org/w/index.php?curid=1679336

Rogers & McClelland, 2003

Multipotential representation learning

- Animals can recombine their existing knowledge to exploit new opportunities

- In machine learning systems, this ability can emerge at scale (e.g., in context learning)

- What are the factors that give rise to *multipotential* representations?

Conclusion & outlook

- Depth introduces a hierarchy of saddle points into the loss landscape, yielding a quasi-systematic progression through stages

- Initialization determines whether these saddle points influence dynamics, yielding several learning regimes

- In nonlinear networks, pathways race to explain the dataset

References

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