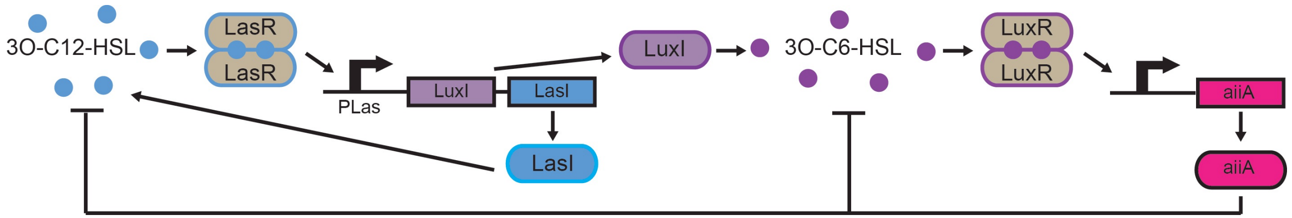
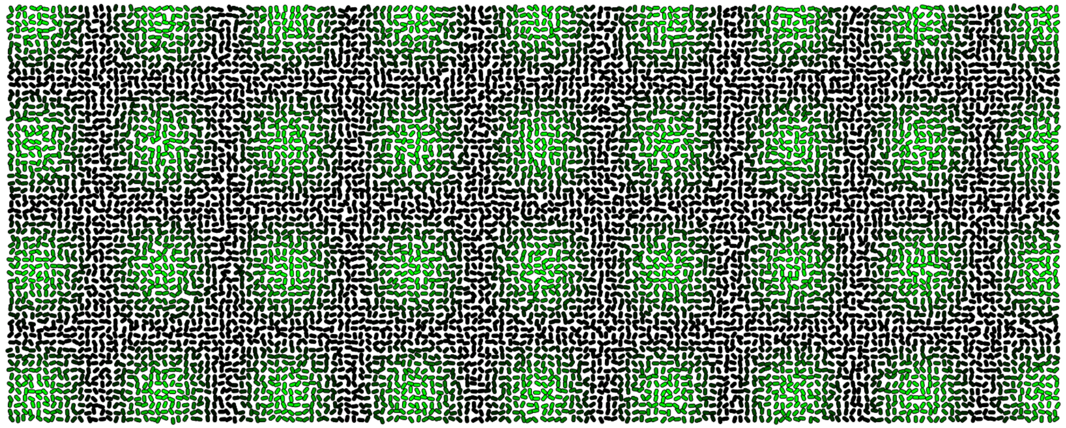
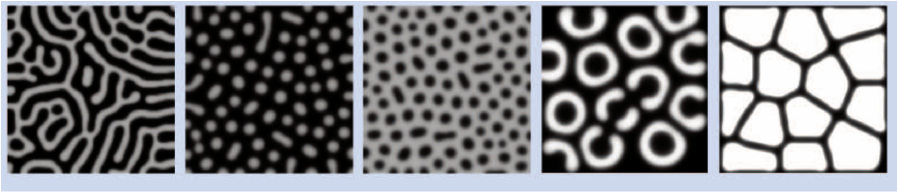
Title: Efficient Amortised Bayesian Inference for Hierarchical and Nonlinear Dynamical Systems







e.g. *Turing* patterns

Motivation: Can we build a synthetic biological systems for **generating patterns**?

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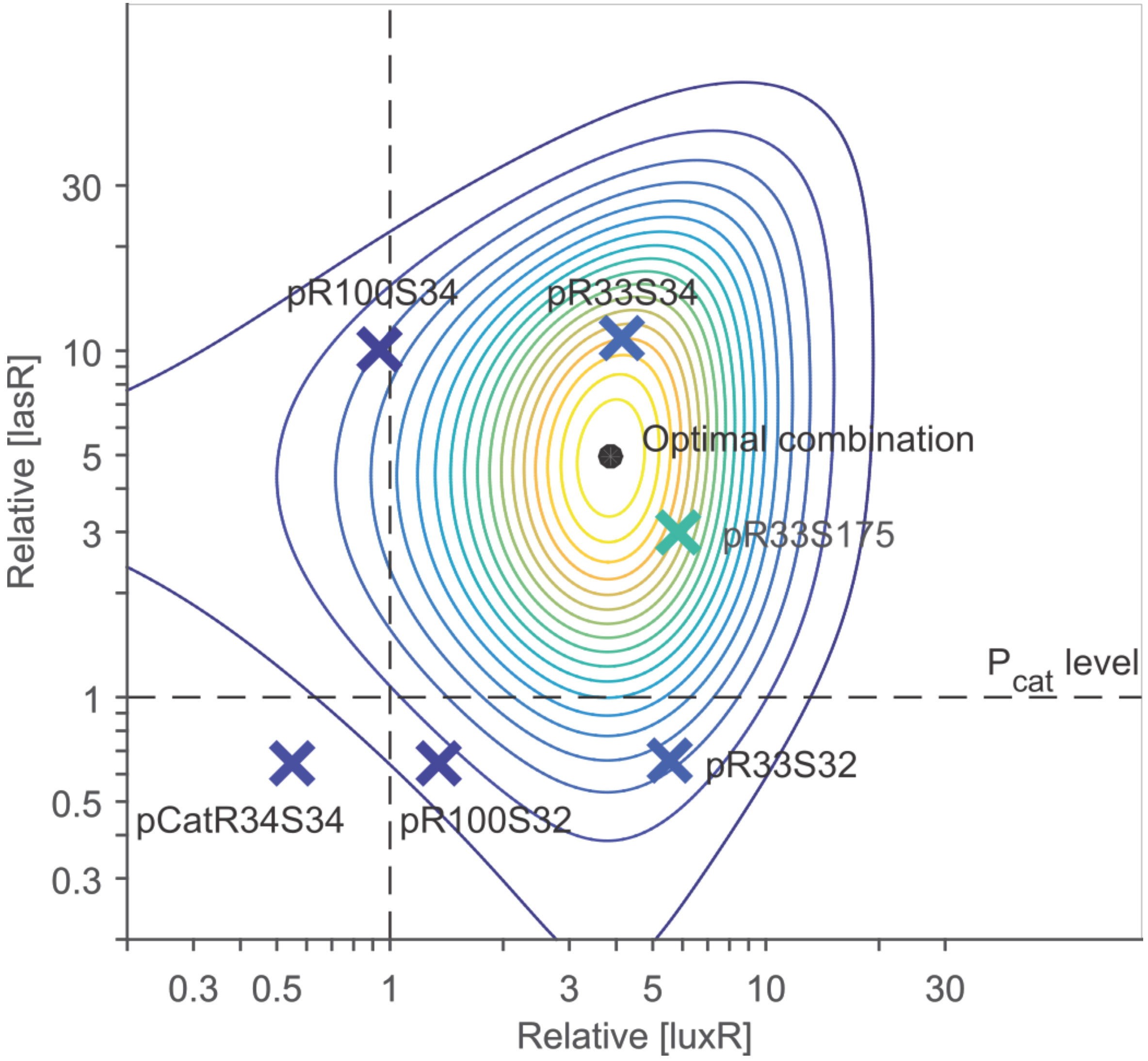
Optimising for Turing Patterns



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Generative Process

$$\mathbf{z} \sim p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{g})$$

Draw ODE parameters, possibly conditioned on group (device components).

$$\dot{\mathbf{x}} = f_{\boldsymbol{\theta}}(\mathbf{x}; \mathbf{z}, \mathbf{u}, \mathbf{g})$$

Define the dynamical system (e.g., ODE)

$$\mathbf{X} = \texttt{Simulate}(f_{\boldsymbol{\theta}}, \mathbf{x}_0)$$

Simulate dynamics (e.g., 2nd order Runge-Kutta)

$$\mathbf{M} = \psi(\mathbf{X}), \quad \boldsymbol{\Sigma} = \rho(\mathbf{X}, \mathbf{z})$$

Observer process relates states X to observations Y;
Noise process defines data variance at each time.

$$\mathbf{Y} \sim p(\mathbf{Y}|\mathbf{M}, \boldsymbol{\Sigma})$$

Likelihood function. Typically Gaussian.

Variational Auto-Encoders for Hierarchical Dynamical Systems

Block-conditional Latent Variables

$$q_{\phi}(\mathbf{z}|\mathbf{Y},\mathbf{g},\mathbf{u}) = \underbrace{q_{\phi_P}(\mathbf{z}_P)}_{\text{Population}} \underbrace{q_{\phi_I}(\mathbf{z}_I|\mathbf{Y},\mathbf{g})}_{\text{Individual}} \underbrace{\prod_j q_{\phi_G^{(j)}}\left(\mathbf{z}_G^{(j)}|\mathbf{g}\right)}_{\text{Group}}$$

ELBO

$$\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{Y},\mathbf{g},\mathbf{u})}[\log p_{\boldsymbol{\theta}}(\mathbf{Y}|\mathbf{z},\mathbf{g},\mathbf{u}) + \log p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{g}) - \log q_{\phi}(\mathbf{z}|\mathbf{Y},\mathbf{g})]$$

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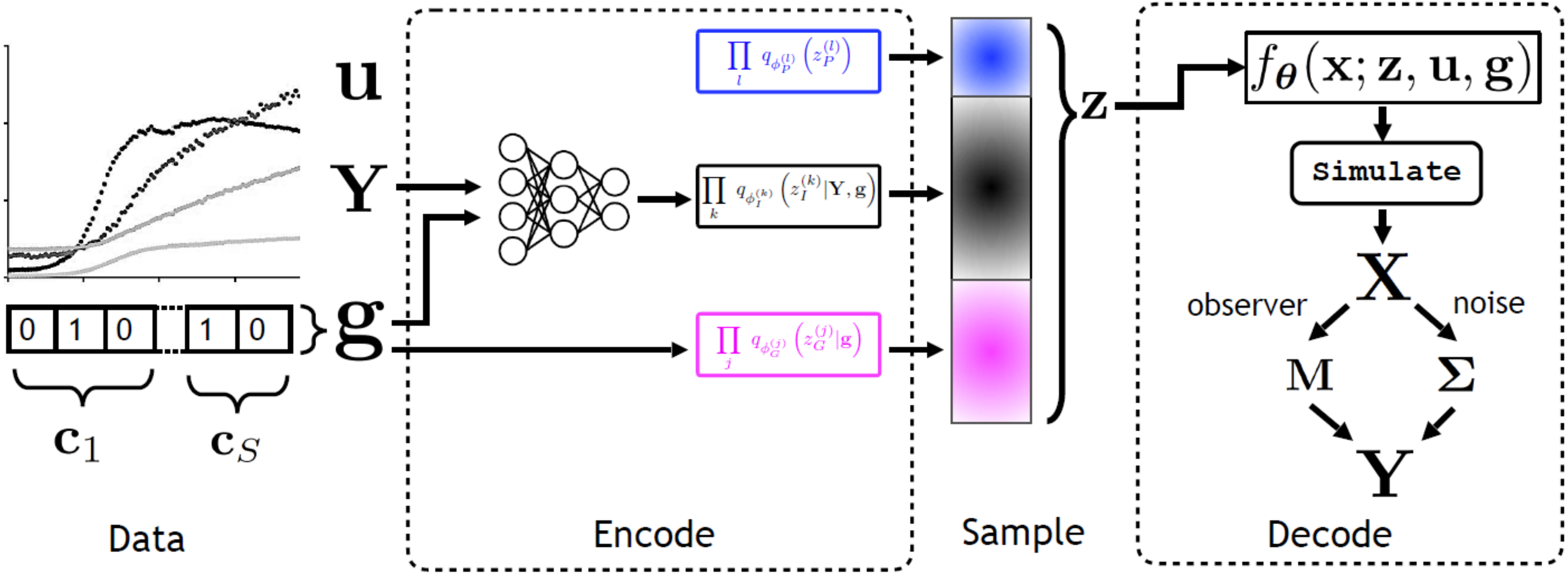
Computational flow diagram



Choice of f_θ : White or Black Box ODEs

White Box

$$\dot{[RFP]} = 1 - (d_{RFP} + \gamma(c)).[RFP]$$

$$\dot{[CFP]} = a_{CFP}.f_{76}(C_6, C_{12}, [R], [S]) - (d_{CFP} + \gamma(c)).[CFP]$$

$$\dot{[YFP]} = a_{YFP}.f_{81}(C_6, C_{12}, [R], [S]) - (d_{YFP} + \gamma(c)).[YFP]$$

$$\dot{[R]} = a_R - (d_R + \gamma(c)).[R]$$

$$\dot{[S]} = a_S - (d_S + \gamma(c)).[S]$$

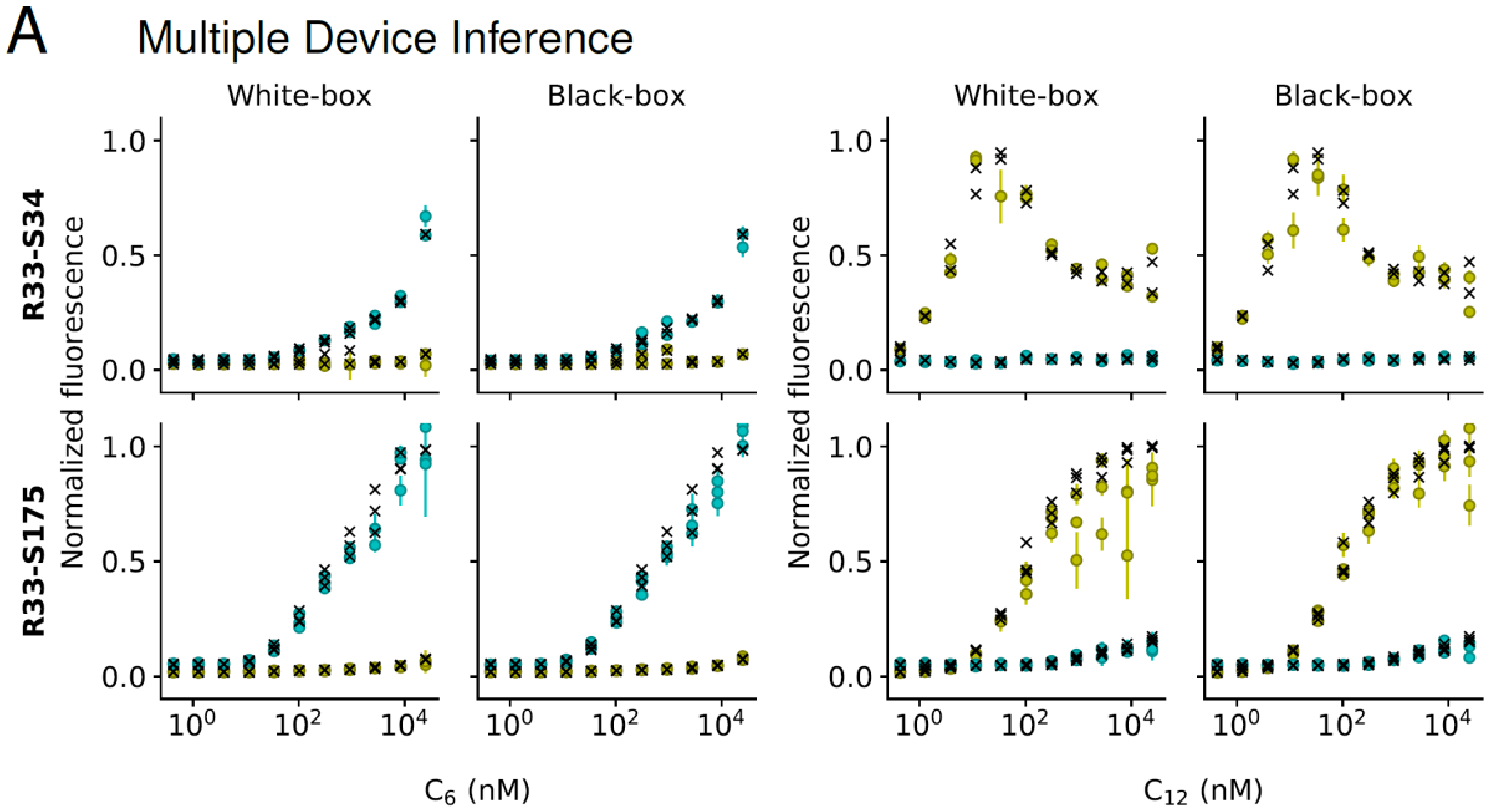
$$\dot{[F_{480}]} = a_{480} - \gamma(c).[F_{480}]$$

$$\dot{[F_{530}]} = a_{530} - \gamma(c).[F_{530}]$$

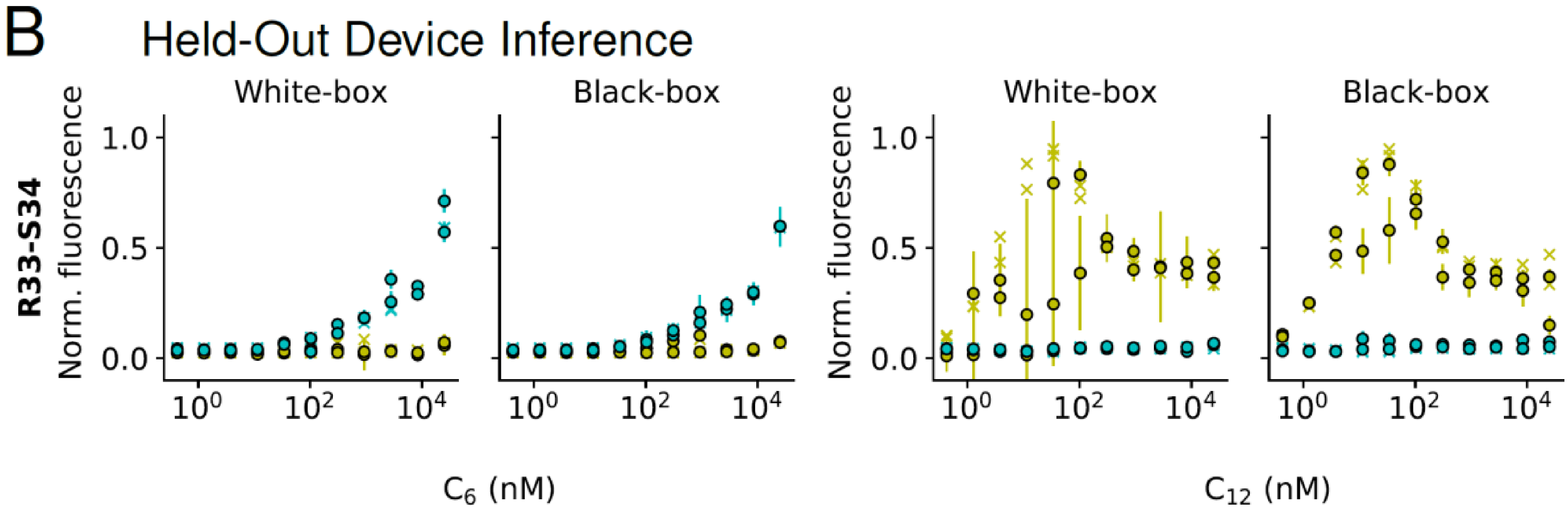
Black Box

$$\dot{\mathbf{x}} = \omega_1^+(\mathbf{x}, \mathbf{\Psi}) - \mathbf{x} \odot \omega_2^+(\mathbf{x}, \mathbf{\Psi})$$

Results: excellent model fit



“Zero-shot” learning on new devices.



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