Learning **physical concepts** purely from data: We demonstrate how **generative models** can learn **manifolds** of **differential equations.**

Rodent: Relevance determination in ODE

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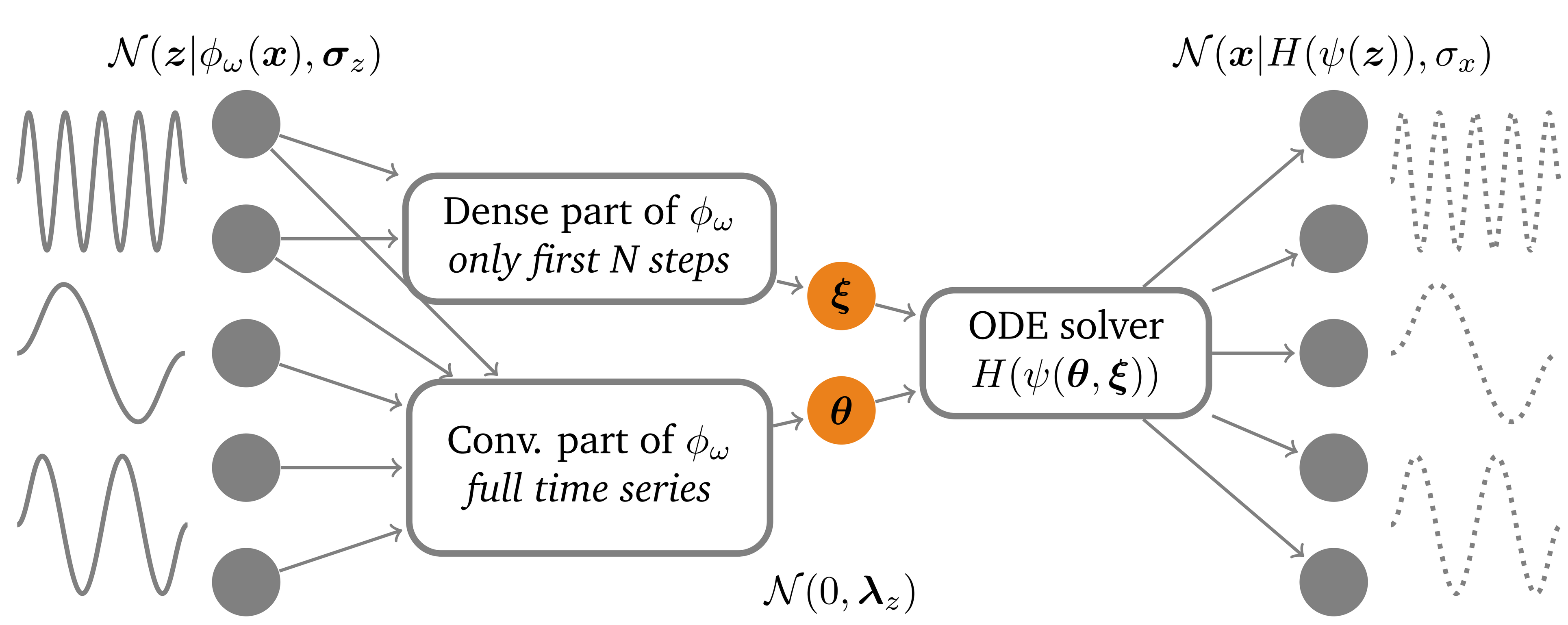
Learning differential equations

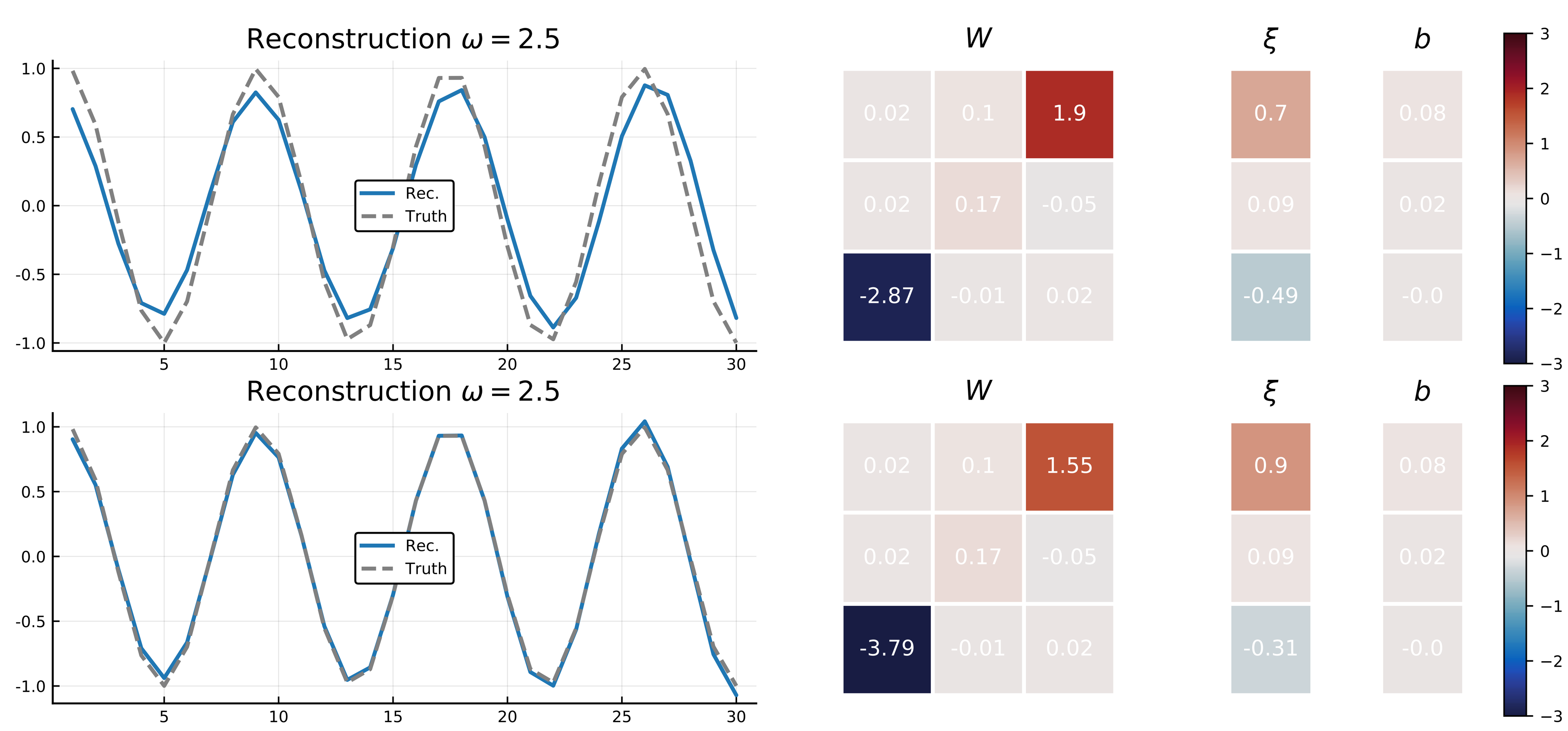
- We want to find the simplest ODE that describes a dynamical system
- By simple we mean: minimal order of ODE and minimum number of non-zero parameters.
- Discover physically meaningful equations that might help understand the underlying process.
- We can learn manifolds of generating models not only a single process



Advantages of the relevant ODE identifier

- **Explainability.** The parameters of z are decoded through an ODE solver, which gives them physical meaning.
- **Sparsity.** The automatic relevance determination prior on z encourages the simplest solution with fewest non-zero parameters.
- **Partial observations.** Rodent allows learning of an ODE without knowledge of all state trajectories. The observation operator is assumed to be known.
- **Time series.** The convolutional part of the encoder is agnostic to different time series lengths.

Manifold learning & Reidentification



Rodent reconstructions (left column) and latent codes (right column) of a harmonic signal in the upper plots. Reidentified reconstruction and encodings in the bottom. The values of the latent codes only change were the variable was detected as relevant. The heatmaps on the right show the corresponding encodings for the weights $\boldsymbol{W}$, biases $\boldsymbol{b}$, and initial conditions $\boldsymbol{\xi}$. The Rodent reduced the latent space to the four truly relevant parameters.

Rodent in depth

Assume a time series $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_K]$ with $\boldsymbol{x}_i \in \mathbb{R}^d$ generated from discrete-time, noisy observations

$$\boldsymbol{x}_k = H(\boldsymbol{\xi}(\Delta t k)) + e_k, \tag{1}$$

where $k = 1 \dots K$, $e_k \sim \mathcal{N}(0, \sigma_e^2 \mathbf{I})$, and partial obs. operator H. The evolution of $\boldsymbol{\xi}(t) \in \mathbb{R}^N$ is governed by an ODE:

$$\frac{\partial \boldsymbol{\xi}}{\partial t} = f(\boldsymbol{\theta}, t) \approx \boldsymbol{W}\boldsymbol{\xi} + \boldsymbol{b}. \tag{2}$$

We aim to learn structure and order of the ODE from a set of trajectories $\{\boldsymbol{X}_i\}_{i=1}^L$ generated by the same generative process but with different $\boldsymbol{\theta}_i$ and different $\boldsymbol{\xi}_i(0)$, for each trajectory, i.e.

$$\boldsymbol{X}_i = H(\psi(\boldsymbol{\theta}_i, \boldsymbol{\xi}_i(0), \boldsymbol{t})) + \boldsymbol{e}, \tag{3}$$

where $\boldsymbol{t} = [0, \Delta t, \dots, K\Delta t]$ and ODE solver ψ. Assuming we observe a system with expected order M, we choose $N \geq M$.

If ODE state and parameters are combined in $\boldsymbol{z} = [\boldsymbol{\theta}, \boldsymbol{\xi}(0)]$ the likelihood becomes

$$p(\boldsymbol{x}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{x}|H(\psi(\boldsymbol{z})), \sigma_x^2). \tag{4}$$

To determine the structure of the ODE, we employ the ARD prior:

$$p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z}|0, \mathrm{diag}(\boldsymbol{\lambda}_z^2)) \quad p(\boldsymbol{\lambda}_z) = 1/\boldsymbol{\lambda}_z. \tag{5}$$

The posterior of $\boldsymbol{z}$ is prescribed by

$$p(\boldsymbol{z}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{z}|\phi_\omega(\boldsymbol{x}), \boldsymbol{\sigma}_z^2) \tag{6}$$

where mean $\boldsymbol{\mu}_z = \phi_\omega(\boldsymbol{x})$ is a NN with parameters ω. The resulting ELBO:

$$\mathcal{L} = \sum_{i=1}^{n} \mathsf{E}_{p(z|x)} \left[\frac{(\boldsymbol{x}_i - \psi(\phi_\omega(\boldsymbol{x}_i) + \boldsymbol{\sigma}_z \odot \boldsymbol{\epsilon}))^2}{2\sigma_e^2} \right] + \frac{nd}{2}\log(\sigma_e) + \sum_{i=1}^{n} \left(\log\left(\frac{\boldsymbol{\lambda}_z^2}{\boldsymbol{\sigma}_z^2}\right) - m + \frac{\boldsymbol{\sigma}_z^2}{\boldsymbol{\lambda}_z^2} + \frac{\phi_\omega(\boldsymbol{x}_i)^2}{\boldsymbol{\lambda}_z^2} \right), \tag{7}$$

with gaussian noise $\boldsymbol{\epsilon}$, decoder $H(\psi(\boldsymbol{\theta}, \boldsymbol{\xi}(0))) \equiv \phi(\boldsymbol{z})$, and $\dim(\boldsymbol{z}) = m$. The encoder network consists of two parts: (i) A dense network that receives only a few steps of the beginning of the time series, responsible for predicting $\boldsymbol{\xi}(0)$. (ii) A (CNN) that predicts $\boldsymbol{\theta}$. The CNN averages over the time dimension after the convolutions, which makes it possible to use samples of different length.

Reidentification. During reidentification we sample a batch of latent codes from the encoder for each input sample. The latent samples are used as starting points for another optimization of the reconstruction error, while keeping all irrelevant parameters fixed. On the left, four parameters, namely W_{13}, W_{31}, ξ_1, and ξ_3, were found to be relevant, so only those are changing during the optimization with respect to R. This means that we stay in the identified model manifold, but are able to extrapolate far beyond the training range.

Check out the full paper at `http://tiny.cc/f6x6gz` or scan the QR code on the left!

Inspired by `#betterposter` by Mike Morrison

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