ODE²VAE: Deep generative second order ODEs with Bayesian neural networks

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Motivation and Previous Work

Task: Learning low-rank latent representations of high dimensional data sequences

Existing techniques:

- ☹ VAEs are mostly for **static** data like images [1].
- ☹ RNN-based VAEs are discrete and fail to produce accurate **long-term** forecasts.
- ☹ Neural ODEs are **first-order**, no regularization [2].

$$\dot{\mathbf{z}}_t := \frac{d\mathbf{z}_t}{dt} = \underbrace{\mathbf{f}(\mathbf{z}_t)}_{\text{NN}}, \qquad \mathbf{z}_T = \mathbf{z}_0 + \int_0^T \mathbf{f}(\mathbf{z}_t)dt$$

We propose:

- ☺ Second-order ODE with **position $\mathbf{s}_t$** and **momentum $\mathbf{v}_t$** latent spaces.
- ☺ **Probabilistic ODEs** with Bayesian neural network differential function.

$$\begin{aligned}\dot{\mathbf{s}}_t &= \mathbf{v}_t \\ \dot{\mathbf{v}}_t &= \underbrace{\mathbf{f}_{\mathcal{W}}(\mathbf{s}_t,\mathbf{v}_t)}_{\text{Bayesian NN}}\end{aligned} \qquad \begin{bmatrix}\mathbf{s}_T \\ \mathbf{v}_T\end{bmatrix} = \begin{bmatrix}\mathbf{s}_0 \\ \mathbf{v}_0\end{bmatrix} + \int_0^T \begin{bmatrix}\mathbf{v}_t \\ \mathbf{f}_{\mathcal{W}}(\mathbf{s}_t,\mathbf{v}_t)\end{bmatrix} dt$$

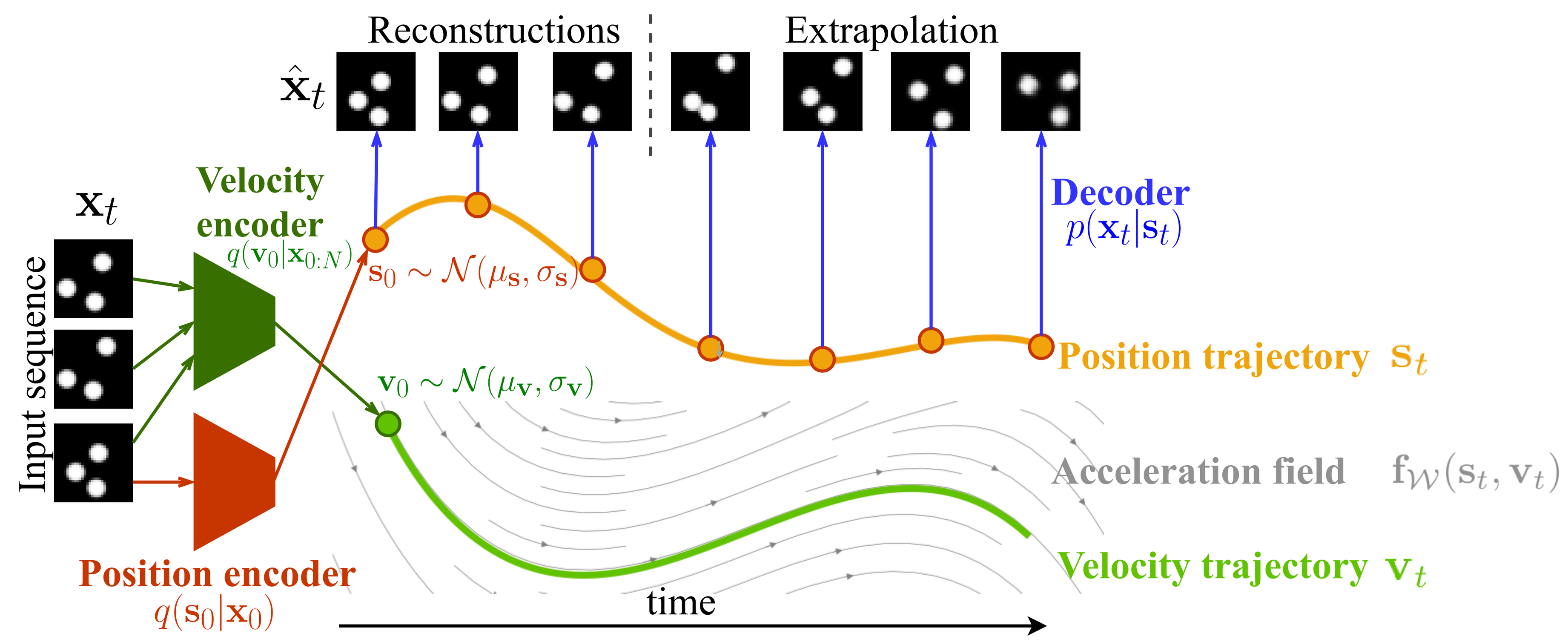
Variational Inference

Denote by $\mathbf{x}_{0:N}$ an observed sequence, $\mathbf{z}_t := (\mathbf{s}_t, \mathbf{v}_t)$ combined state, $\mathcal{W}$ weights of differential neural network $\mathbf{f}_{\mathcal{W}}(\mathbf{s},\mathbf{v})$, and $q(\mathcal{W}, \mathbf{z}_{0:N}|\mathbf{x}_{0:N}) = q(\mathcal{W}) q_{\text{enc}}(\mathbf{z}_0|\mathbf{x}_{0:N}) q_{\text{ode}}(\mathbf{z}_{1:N}|\mathbf{x}_{0:N}, \mathbf{z}_0, \mathcal{W})$ the variational posterior. Then, ELBO becomes

$$\begin{aligned}\mathcal{L} = &-\text{KL}[q(\mathcal{W})||p(\mathcal{W})] && \texttt{\# ODE penalty} \\ &-\text{KL}[q_{\text{enc}}(\mathbf{z}_0|\mathbf{x}_{0:N})||p(\mathbf{z}_0)] && \texttt{\# VAE penalty} \\ &-\sum_i \mathbb{E}_{q(\mathcal{W})}[\text{KL}[q_{\text{ode}}(\mathbf{z}_i|\mathcal{W},\mathbf{x}_{0:N})||p(\mathbf{z}_i)]] && \texttt{\# dynamic penalty} \\ &+\mathbb{E}_{q_{\text{enc}}(\mathbf{z}_0|\mathbf{x}_{0:N})}[\log p(\mathbf{x}_0|\mathbf{z}_0)] && \texttt{\# VAE reconstr.} \\ &+\sum_i \mathbb{E}_{q(\mathcal{W})}\mathbb{E}_{q_{\text{ode}}(\mathbf{z}_i|\mathbf{x}_{0:N},\mathbf{z}_0,\mathcal{W})}[\log p(\mathbf{x}_i|\mathbf{z}_i)] && \texttt{\# dynamic reconstr.}\end{aligned}$$

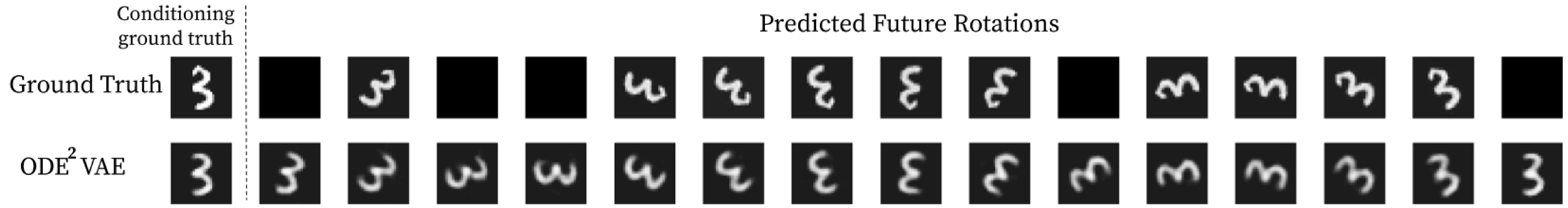
Generative Model

$$\begin{aligned}&\mathbf{s}_0 \sim p(\mathbf{s}_0) && \texttt{\# position encoder} \\ &\mathbf{v}_0 \sim p(\mathbf{v}_0) && \texttt{\# velocity encoder} \\ &\mathbf{s}_t = \mathbf{s}_0 + \int_0^t \mathbf{v}_\tau d\tau && \texttt{\# position trajectory} \\ &\mathbf{v}_t = \mathbf{v}_0 + \int_0^t \mathbf{f}_{\text{true}}(\mathbf{s}_\tau, \mathbf{v}_\tau) d\tau && \texttt{\# velocity trajectory} \\ &\mathbf{x}_i \sim p(\mathbf{x}_i|\mathbf{s}_i), \quad i \in [0, N] && \texttt{\# decoder}\end{aligned}$$



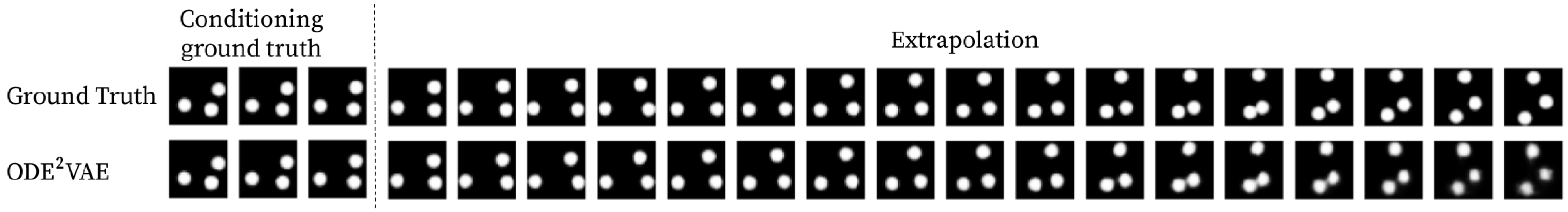
Rotating MNIST Experiment

Dataset: Sequences of rotating handwritten 3s with 30% missing data (black squares below).



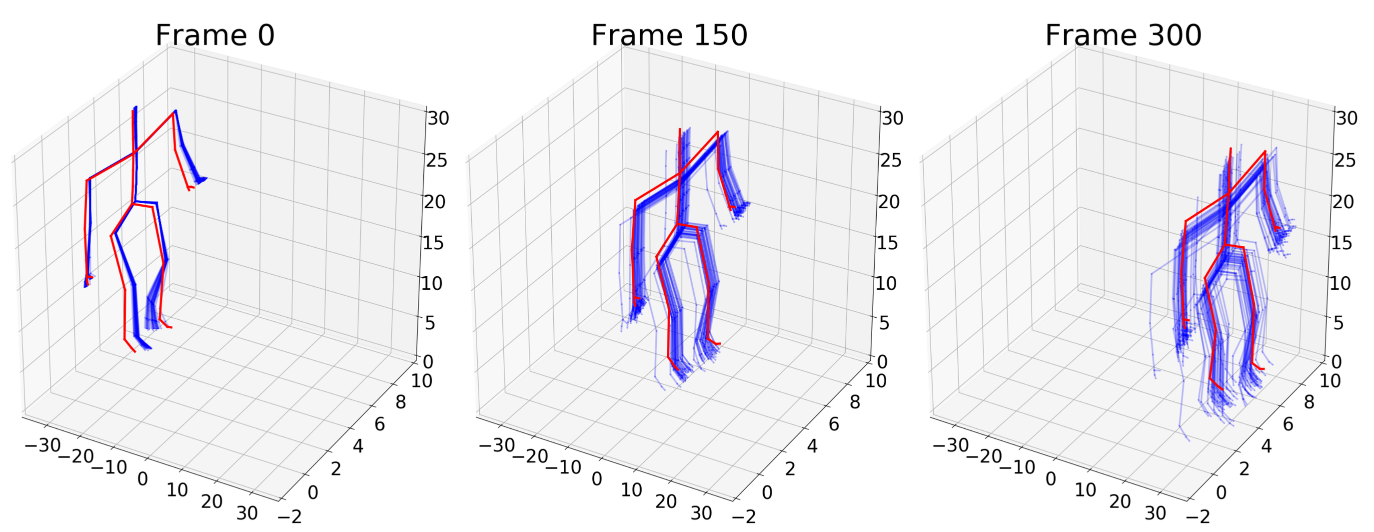
Bouncing Balls Experiment

Dataset: Sequences of three balls bouncing within a box (50 frames of size 32x32 per sequence)



CMU Walking Data Experiment

- 62-dim sensor measurements
- 12 training sequences
- 300 frames per sequence
- Red is a test sequence and blues are 30 draws from learned model, conditioned on first 3 frames



References

[1] Kingma, Diederik P., and Max Welling. "Auto-encoding variational bayes." arXiv preprint arXiv:1312.6114 (2013).

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