

# Dynamical Variational Autoencoders

## Links to stochastic differential equations

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# Summary

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# Abstract

- **Variational Auto Encoders (VAEs)** have limitations when dealing with data sequences, due to i.i.d assumption.
- **Dynamical Variational Auto Encoders ([10])** are adapted to data sequences
  - Temporal dependency built into latent prior
  - Discrete or continuous time prior
  - Observation model as in regular VAEs: Gaussian, Bernoulli, Student-t...
- **Link to Stochastic Calculus**
  - Solutions to linear Stochastic Differential Equations (SDEs) are Gaussian processes : run prior Gaussian Process (GP) regression at linear cost.
  - Solutions to general SDEs are Markov processes : link to more general Latent Stochastic Differential Equation models (Latent SDEs)
- **What we will cover today**
  - General theory of Dynamical Variational Auto Encoders (DVAEs)
  - Review of some discrete and continuous time DVAEs with XPs : Deep Kalman Filter (DKF), Variational Recurrent Neural Network (VRNN), Gaussian Process Variational Auto Encoder (GP-VAE)
  - Stochastic calculus survival kit
  - Relationships between DVAEs and stochastic calculus
  - Early perspective on Latent Ordinary Differential Equation models (Latent ODEs) and Latent SDEs

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# Dynamical Variational Auto Encoders : generalities

- Time : regular  $t_1, t_2, \dots, t_T$  or irregular  $t_{i_1}, t_{i_2}, \dots, t_{i_T}$  sampling times
- Observations : a sequence of  $T$  points  $x_{1:T} = \{(x_t)_{t=1, \dots, T}\}$  (or  $x_{t_1:t_T} = \{(x_{t_i})_{i=1, \dots, T}\} \in \mathbb{R}^F$ ).
- Latent variables : an associated sequence of  $T$  latent variables  $z_{1:T} = \{(z_t)_{t=1, \dots, T}\} \in \mathbb{R}^L$  (resp.  $z_{t_1}, \dots, z_{t_T}$ )
- Optionally, a sequence of -usually deterministic-  $T$  inputs  $u_{1:T} = \{(u_t)_{t=1, \dots, T}\} \in \mathbb{R}^U$  (resp.  $u_{t_i}, i = 1, \dots, T$ )
- Encoding temporal dependency in prior over  $z_i$ 's
- Arbitrary likelihood (observation model)
- Approximate posterior usually same form as true posterior
- Use D-Separation in Graphical Probabilistic Model (GPM) to simplify expressions
- Untractable true posterior  $\implies$  training by maximizing a Variational Lower Bound (VLB)

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## General formulation of DVAE

### Generative model

$$\begin{aligned} p(x_{1:T}, z_{1:T} | u_{1:T}) &= \prod_{t=1}^T p(x_t, z_t | x_{1:t-1}, z_{1:t-1}, u_{1:T}) \\ &= \prod_{t=1}^T p(x_t | x_{1:t-1}, z_{1:t}, u_{1:T}) p(z_t | x_{1:t-1}, z_{1:t-1}, u_{1:T}) \\ &= \prod_{t=1}^T p(x_t | x_{1:t-1}, z_{1:t}, u_{1:t}) p(z_t | x_{1:t-1}, z_{1:t-1}, u_{1:t}) \end{aligned}$$

**Only assumption : causal dependency  $x_t, z_t$  on inputs  $u_{1:t} \implies |u_{1:T} = |u_{1:t}$ .**  
(NB : assume no input in the rest of the presentation)

# Posteriors

- True posterior  $p(z_{1:T}|x_{1:T})$  usually untractable::

$$p(z_{1:T}|x_{1:T}) = \prod_{t=1}^T p(z_t|z_{1:t-1}, x_{1:T})$$

- Inference model : approximate posterior by an parametric encoder  $q_\phi(z_{1:T}|x_{1:T})$  ( $\phi$  the set of parameters):

$$q_\phi(z_{1:T}|x_{1:T}) = \prod_{t=1}^T q_\phi(z_t|z_{1:t-1}, x_{1:T})$$

- D-separation on GPM to simplify  $p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t})$  and  $q_\phi(z_t|z_{1:t-1}, x_{1:T})$
- Good practice : use the true posterior expression  $p(z_{1:T}|x_{1:T})$  for  $q_\phi(z_t|z_{1:t-1}, x_{1:T})$

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# Likelihood

- Observation model and encoder:

$$p_{\theta}(x_{1:T}, z_{1:T}) = \prod_{t=1}^T p_{\theta_x}(x_t | x_{1:t-1}, z_{1:t}) p_{\theta_z}(z_t | z_{1:t-1}, x_{1:t-1}) \quad (1)$$

$$q_{\phi}(z_{1:T} | x_{1:T}) = \prod_{t=1}^T q_{\phi}(z_t | z_{1:t-1}, x_{1:T}) \quad (2)$$

- Log likelihood

$$\log p(x_{1:T}) = \log \frac{p(x_{1:T}, z_{1:T})}{p(z_{1:T} | x_{1:T})} \quad (3)$$

$$= \mathbb{E}_{q_{\phi}(z_{1:T} | x_{1:T})} \log \frac{p(x_{1:T}, z_{1:T})}{q_{\phi}(z_{1:T} | x_{1:T})} \frac{q_{\phi}(z_{1:T} | x_{1:T})}{p(z_{1:T} | x_{1:T})} \quad (4)$$

$$= \mathbb{E}_{q_{\phi}(z_{1:T} | x_{1:T})} \log \frac{p(x_{1:T}, z_{1:T})}{q_{\phi}(z_{1:T} | x_{1:T})} + \text{KL}(q_{\phi}(z_{1:T} | x_{1:T}) || p(z_{1:T} | x_{1:T})) \quad (5)$$

$$\geq \mathbb{E}_{q_{\phi}(z_{1:T} | x_{1:T})} \log \frac{p(x_{1:T}, z_{1:T})}{q_{\phi}(z_{1:T} | x_{1:T})} = \mathcal{L}(\theta, \phi, X) \quad (6)$$

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## Variational Lower Bound

- Lower bound:

$$\mathcal{L}(\theta, \phi, X) = \mathbb{E}_{q_\phi(z_{1:T}|x_{1:T})} \log \left( \frac{\prod_{t=1}^T p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}) p_{\theta_z}(z_t|z_{1:t-1}, x_{1:t-1})}{\prod_{t=1}^T q_\phi(z_t|z_{1:t-1}, x_{1:T})} \right) \quad (7)$$

$$= \mathbb{E}_{q_\phi(z_{1:T}|x_{1:T})} \left( \sum_{t=1}^T \log p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}) - \sum_{t=1}^T \log \frac{q_\phi(z_t|z_{1:t-1}, x_{1:T})}{p_{\theta_z}(z_t|z_{1:t-1}, x_{1:t-1})} \right) \quad (8)$$

$$= \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{1:t}|x_{1:T})} \log p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}) - \quad (9)$$

$$\sum_{t=1}^T \mathbb{E}_{q_\phi(z_{1:t-1}|x_{1:T})} \mathbb{KL} (q_\phi(z_t|z_{1:t-1}, x_{1:T}) || p_{\theta_z}(z_t|z_{1:t-1}, x_{1:t-1})) \quad (10)$$

- First term : often called **reconstruction error** (formally a log likelihood)
- Second term : **regularization term**, average divergence between the approximate posterior distribution at time  $t$ , and its real distribution.
- Sampling over  $q_\phi$  requires the "re-parametrization trick" (see [11]), for  $\mathcal{L}(\theta, \phi, X)$  to be differentiable w.r.t.  $\theta, \phi$ .

## Summary DVAE

General Dynamical VAEs : generative and inference models; variational lower bound

$$p(x_{1:T}, z_{1:T}) = \prod_{t=1}^T p_{\theta_x}(x_t | x_{1:t-1}, z_{1:t}) p_{\theta_z}(z_t | z_{1:t-1}, x_{1:t-1}) \quad (11)$$

$$q_\phi(z_{1:T} | x_{1:T}) = \prod_{t=1}^T q_\phi(z_t | z_{1:t-1}, x_{1:T}) \quad (12)$$

$$\begin{aligned} \mathcal{L}(\theta, \phi, X) &= \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{1:t} | x_{1:T})} \log p_{\theta_x}(x_t | x_{1:t-1}, z_{1:t}) \\ &\quad - \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{1:t-1} | x_{1:T})} \mathbb{KL}(q_\phi(z_t | z_{1:t-1}, x_{1:T}) || p_{\theta_z}(z_t | z_{1:t-1}, x_{1:t-1})) \end{aligned} \quad (13)$$

## First model : Deep Kalman Filter

Deep Kalman Filter Directed Acyclic Graph (DAG): State Space Model (SSM) with Gaussian likelihood parameterized by neural nets.

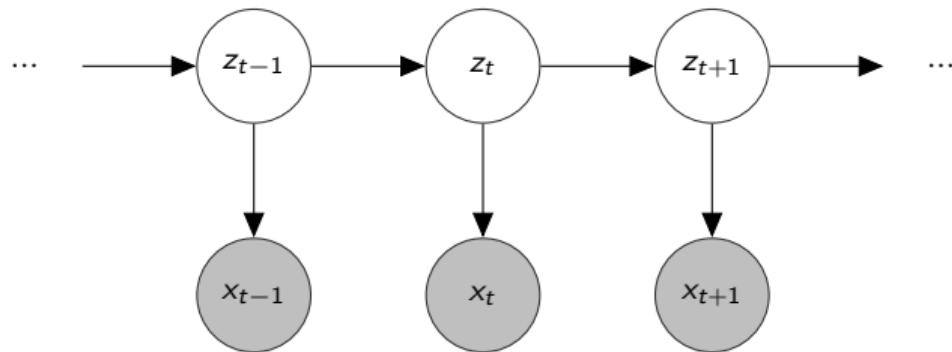


Figure: Probabilistic model of a Deep Kalman Filter

## Deep Kalman Filter - generative model

- Use **D-separation** ([1], [13], [17]) to simplify the general DVAE expressions 11 and 12.
- Conditioning on  $z_t$  and  $z_{t-1}$  drives:

$$p_{\theta_x}(x_t | x_{1:t-1}, z_{1:t}) = p_{\theta_x}(x_t | z_t) \quad (14)$$

$$p_{\theta_z}(z_t | z_{1:t-1}, x_{1:t}) = p_{\theta_z}(z_t | z_{t-1}) \quad (15)$$

$$q_{\phi}(z_t | z_{1:t-1}, x_{1:T}) = q_{\phi}(z_t | z_{t-1}, x_{t:T}) \quad (16)$$

## Deep Kalman Filter - generative model - 2

- Gaussian distributions for  $p_{\theta_x}$ ,  $p_{\theta_z}$  and  $q_\phi$  (mean and diagonal covariance learnt by neural networks).

$$p_{\theta_x}(x_t|z_t) = \mathcal{N}(x_t|\mu_{\theta_x}(z_t), \text{diag } \sigma_{\theta_x}^2(z_t)) \quad (17)$$

$$p_{\theta_z}(z_t|z_{t-1}) = \mathcal{N}(z_t|\mu_{\theta_z}(z_{t-1}), \text{diag } \sigma_{\theta_z}^2(z_{t-1})) \quad (18)$$

$$q_\phi(z_t|z_{t-1}, x_{t:T}) = \mathcal{N}(z_t|\mu_\phi(z_{t-1}, x_{t:T}), \text{diag } \sigma_{\theta_z}^2(z_{t-1}, x_{t:T})) \quad (19)$$

- Some other formulations of the approximate posterior (encoder) are possible. For example:

$$q_\phi(z_t|z_{t-1}, x_t)$$

$$q_\phi(z_t|z_{1:t}, x_{1:t})$$

$$q_\phi(z_t|z_{1:T}, x_{1:T})$$

- We have chosen 16 for the implementation (same form as the true posterior).

## Deep Kalman Filter - ELBO

Using D-Separation, the Evidence Lower Bound (ELBO) 13 simplifies into:

$$\mathcal{L}(\theta, \phi, X) = \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{1:t}|x_{1:T})} \log p_{\theta_x}(x_t|z_t) - \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{1:t-1}|x_{1:T})} \mathbb{KL}(q_\phi(z_t|z_{t-1}, x_{t:T}) || p_{\theta_z}(z_t|z_{t-1})) \quad (20)$$

$$= \sum_{t=1}^T \mathbb{E}_{q_\phi(z_t|x_{1:T})} \log p_{\theta_x}(x_t|z_t) - \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{t-1}|x_{1:T})} \mathbb{KL}(q_\phi(z_t|z_{t-1}, x_{t:T}) || p_{\theta_z}(z_t|z_{t-1})) \quad (21)$$

# Deep Kalman Filter - summary

## Deep Kalman Filter

- **generative model**

$$p_{\theta_x}(x_t|z_t) = \mathcal{N}(x_t|\mu_{\theta_x}(z_t), \text{diag } \sigma_{\theta_x}^2(z_t)) \quad (22)$$

$$p_{\theta_z}(z_t|z_{t-1}) = \mathcal{N}(z_t|\mu_{\theta_z}(z_{t-1}), \text{diag } \sigma_{\theta_z}^2(z_{t-1})) \quad (23)$$

- **inference model**

$$q_{\phi}(z_t|z_{t-1}, x_{t:T}) = \mathcal{N}(z_t|\mu_{\phi}(z_{t-1}, x_{t:T}), \text{diag } \sigma_{\theta_z}^2(z_{t-1}, x_{t:T})) \quad (24)$$

- **VLB for training**

$$\mathcal{L}(\theta, \phi, X) = \sum_{t=1}^T \mathbb{E}_{q_{\phi}(z_t|x_{1:T})} \log p_{\theta_x}(x_t|z_t) - \sum_{t=1}^T \mathbb{E}_{q_{\phi}(z_{t-1}|x_{1:T})} \mathbb{KL}(q_{\phi}(z_t|z_{t-1}, x_{t:T})||p_{\theta_z}(z_t|z_{t-1})) \quad (25)$$

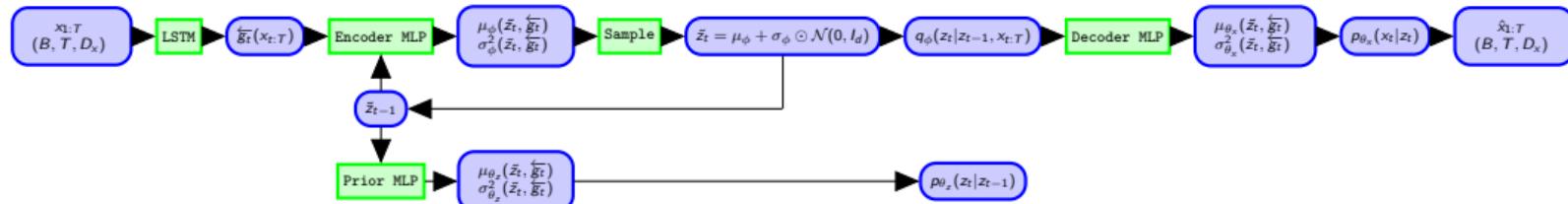
# DKF - Torch

- The  $\text{KL}(q_\phi || p_{\theta_z})$ 's have a close form, as the two distributions are Gaussians.
- Encode  $x_{1:t}$  with forward Long Short Term Memory (LSTM)
- Encode  $x_{t:T}$  with backward LSTM
- Use LSTMs states as inputs to the Multi Layer Perceptron (MLP) parametrizing the distributions.
- For example:

$$\begin{aligned}\overleftarrow{g}_t &= \text{Backward LSTM}(\overleftarrow{g}_{t+1}, x_t) \text{ (encodes } x_{t:T}) \\ q_\phi(z_t | z_{t-1}, x_{t:T}) &= \mathcal{N}(z_t | \mu_\phi(z_{t-1}, \overleftarrow{g}_t), \text{diag } \sigma_\phi^2(z_{t-1}, \overleftarrow{g}_t))\end{aligned}$$

## DKF - Torch - Schematic blocks

The PyTorch implementation is described below:



$$\mathcal{L}(\theta, \phi, X) = \sum_{t=1}^T \mathbb{E}_{q_\phi(z_t | x_{1:T})} \log p_{\theta_x}(x_t | z_t) - \sum_{t=1}^T \mathbb{E}_{q_\phi(z_{t-1} | x_{1:T})} \mathbb{KL}(q_\phi(z_t | z_{t-1}, x_{1:T}) || p_{\theta_z}(z_t | z_{t-1}))$$

## Second model : Variational RNN

- The VRNN is the most expressive DVAE : the general expressions 11, 12 and VLB 13 can not be simplified.
- The GPM of the VRNN assumes full connections between latent variables, and between observed variables.

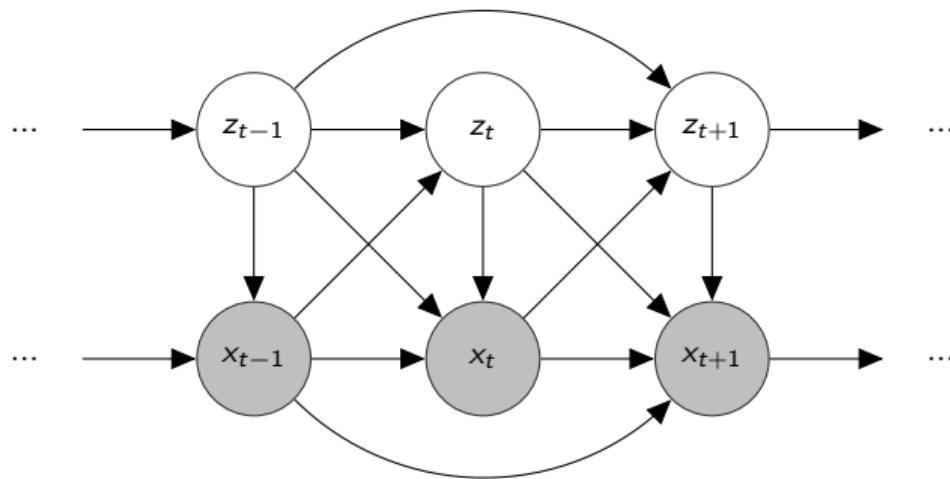


Figure: Probabilistic model of a Variational RNN

# VRNN - Summary

## Variational RNN

- **generative model**

$$p_{\theta_x}(x_t | x_{1:t-1}, z_{1:t}) = \mathcal{N}(x_t | \mu_{\theta_x}(x_{1:t-1}, z_{1:t}), \text{diag } \sigma_{\theta_x}^2(x_{1:t-1}, z_{1:t})) \quad (26)$$

$$p_{\theta_z}(z_t | z_{1:t-1}, x_{1:t-1}) = \mathcal{N}(z_t | \mu_{\theta_z}(z_{1:t-1}, x_{1:t-1}), \text{diag } \sigma_{\theta_z}^2(z_{1:t-1}, x_{1:t-1})) \quad (27)$$

- **inference model**

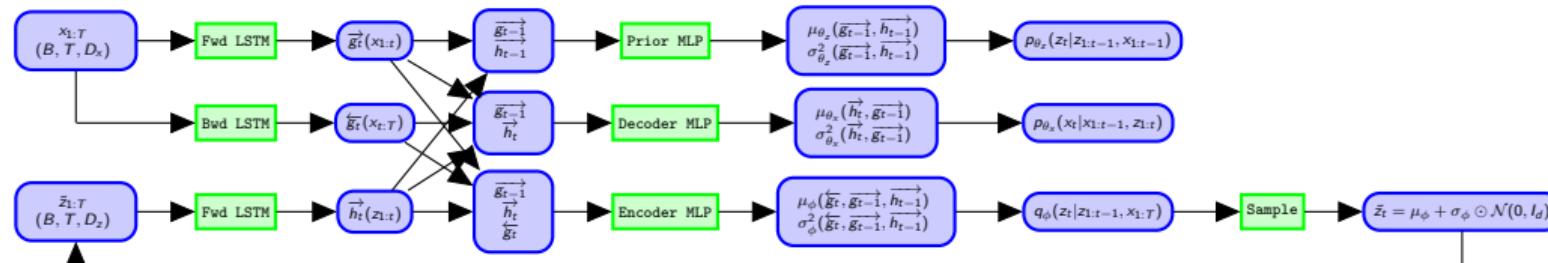
$$q_{\phi}(z_t | z_{1:t-1}, x_{1:T}) = \mathcal{N}(z_t | \mu_{\phi}(z_{1:t-1}, x_{1:T}), \text{diag } \sigma_{\phi}^2(z_{1:t-1}, x_{1:T})) \quad (28)$$

- **VLB for training**

$$\begin{aligned} \mathcal{L}(\theta, \phi, X) &= \sum_{t=1}^T \mathbb{E}_{q_{\phi}(z_{1:t} | x_{1:T})} \log p_{\theta_x}(x_t | x_{1:t-1}, z_{1:t}) \\ &\quad - \sum_{t=1}^T \mathbb{E}_{q_{\phi}(z_{1:t-1} | x_{1:T})} \mathbb{KL}(q_{\phi}(z_t | z_{1:t-1}, x_{1:T}) || p_{\theta_z}(z_t | z_{1:t-1}, x_{1:t-1})) \end{aligned} \quad (29)$$

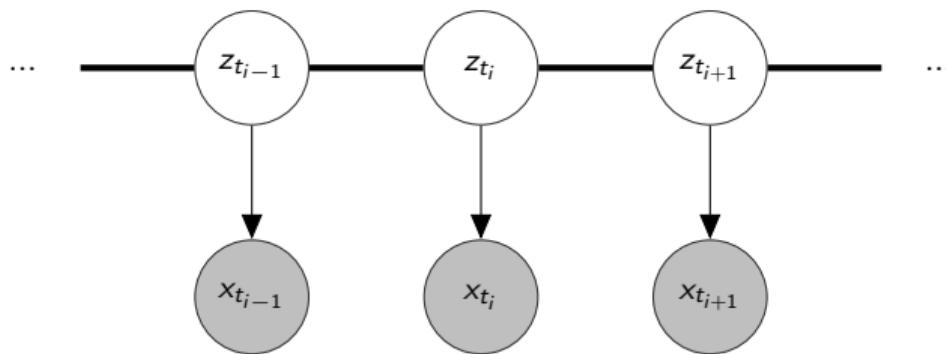
## VRNN - Torch

We have chosen a different implementation from [10] and used three different LSTM networks to encode  $z_{1:t}$ ,  $x_{1:t-1}$  and  $x_{t:T}$  respectively.



$$\mathcal{L}(\theta, \phi, X) = \sum_{t=1}^T \mathbb{E}_{q_{\phi}(z_{1:t}|x_{1:T})} \log p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}) - \sum_{t=1}^T \mathbb{E}_{q_{\phi}(z_{1:t-1}|x_{1:T})} \text{KL}(q_{\phi}(z_t|z_{1:t-1}, x_{1:T}) || p_{\theta_x}(z_t|z_{1:t-1}, x_{1:t-1}))$$

## Third model : Gaussian Process - Variational Auto Encoder



**Figure:** Probabilistic model of a GP-VAE

- **thick black lines** indicate a Gaussian Process prior over latent variables.
- The joint distribution writes:

$$p(x_{t_1:t_T}, z_{t_1:t_T}) = p(z_{t_1:t_T}) \prod_{i=1}^T p(x_{t_i} | z_{t_i}) \quad (30)$$

## GP-VAE generative model

- **Gaussian Process prior** : the prior over the latent variables  $z_{t_i} \in \mathbb{R}^L$  is a set of scalar Gaussian Process over each of the dimension  $l \in \{1, \dots, L\}$  of the latent variables. Formally:

$$p_{\theta_z}(z_{t_1:t_T}^l) = \mathcal{GP}(m_{\theta_z,l}(t_1:t_T), k_{\theta_z,l}(t_1:t_T, t_1:t_T)) \quad l = 1, \dots, L \quad (31)$$

- $m_{\theta_z,l}$  are the  $L$  mean functions of the GP priors (usually chosen constant null)
- $k_{\theta_z,l}$  are the kernel functions of the GP priors. Can be chosen differently to account for prior knowledge of the data sequence.
- Each  $\mathcal{GP}^l$  encode a temporal dependency over  $z^{(l)}$
- Correlation accross dimensions of data is encoded within likelihood  $p_{\theta_x}$

- **Approximate posterior -encoder** :  $q_\phi$  is a set of  $L$  Gaussian distributions of dimension  $T$ , each one accounting for a component of  $z_{t_i}$ . Formally :

$$q_\phi(z_{t_1:t_T}^l | x_{t_1:t_T}^l) = \mathcal{N}(m_\phi^l(x_{t_1:t_T}), \Sigma_\phi^l(x_{t_1:t_T})) \quad l = 1, \dots, L \quad (32)$$

$$= \mathcal{N}(m_\phi^l(x_{t_1:t_T}), \Lambda_\phi^l(x_{t_1:t_T})^{-1}) \quad (33)$$

$$= \mathcal{N}(m_\phi^l(x_{t_1:t_T}), L_\phi^l(x_{t_1:t_T}) L_\phi^l(x_{t_1:t_T})^T) \quad (34)$$

Code covariance with covariance matrix  $\Sigma_\phi^l$ , precision matrix  $\Lambda_\phi^l$ , or with a Cholesky decomposition  $L_\phi^l L_\phi^l$ .

## GP-VAE generative model

From [15]

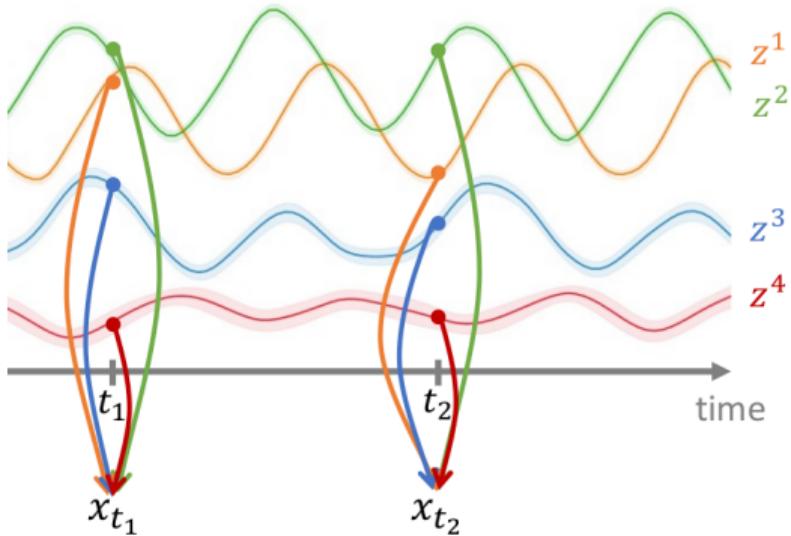


Figure: GP-VAE Schematics

## GP-VAE likelihood and ELBO

$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^T \mathbb{E}_{q_\phi(z_{t_i} | x_{t_1:t_T})} \log p_{\theta_x}(x_{t_i} | z_{t_i}) - \text{KL} (q_\phi(z_{t_1:t_T} | x_{t_1:t_T}) || p_{\theta_z}(z_{t_1:t_T})) \quad (35)$$

We note that:

- the KL-divergence is the sum of the  $L$  KL-divergences  $\text{KL} (q_\phi^l || p_{\theta_z}^l)$  (close form solution)
- the negative log likelihood loss term requires sampling from  $q_\phi(z_{t_i} | x_{t_1:t_T})$  using the reparameterization trick as usual.
- the GP priors  $p_{\theta_z}(z_{t_1:t_T})$  depend only on the time stamps  $t_1, \dots, t_T$ . ( $O(N^3)$  cost)
  - If the kernel parameters are fixed -such as in [8]- then the priors can be computed before the training loop.
  - If the kernel parameters are learnt with the weights of the neural nets (such as in [29]), then the computation must occur at each training iteration.

# GP-VAE Summary

## Gaussian Process VAEs

$$p(x_{t_1:t_T}, z_{t_1:t_T}) = p(z_{t_1:t_T}) \prod_{i=1}^T p(x_{t_i} | z_{t_i}) \quad (36)$$

$$p_{\theta_z}(z_{t_1:t_T}^l) = \mathcal{GP}(m_{\theta_z,l}(t_1:t_T), k_{\theta_z,l}(t_1:t_T)) \quad l = 1, \dots, L \quad (37)$$

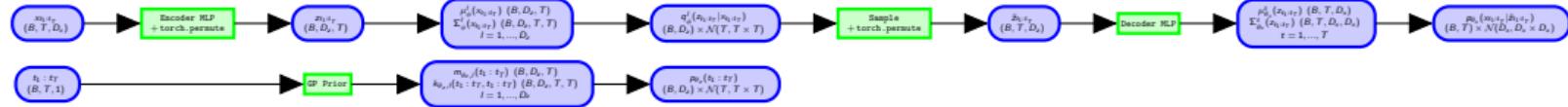
$$q_\phi(z_{t_1:t_T}^l | x_{t_1:t_T}^l) = \mathcal{N}(m_\phi^l(x_{t_1:t_T}), \Sigma_\phi^l(x_{t_1:t_T})) \quad l = 1, \dots, L \quad (38)$$

$$= \mathcal{N}(m_\phi^l(x_{t_1:t_T}), \Lambda_\phi^l(x_{t_1:t_T})^{-1}) \quad (39)$$

$$= \mathcal{N}(m_\phi^l(x_{t_1:t_T}), L_\phi^l(x_{t_1:t_T}) L_\phi^l(x_{t_1:t_T})^T) \quad (40)$$

$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^T \mathbb{E}_{q_\phi(z_{t_i} | x_{t_1:t_T})} \log p_{\theta_x}(x_{t_i} | z_{t_i}) - \mathbb{KL}(q_\phi(z_{t_1:t_T} | x_{t_1:t_T}) || p_{\theta_z}(z_{t_1:t_T})) \quad (41)$$

# GP-VAE - Torch



$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^T \mathbb{E}_{q_\phi(z_{t_i} | x_{t_1:t_T})} \log p_{\theta_X}(x_{t_i} | z_{t_i}) - \text{KL}(q_\phi(z_{t_1:t_T} | x_{t_1:t_T}) || p_{\theta_Z}(z_{t_1:t_T}))$$

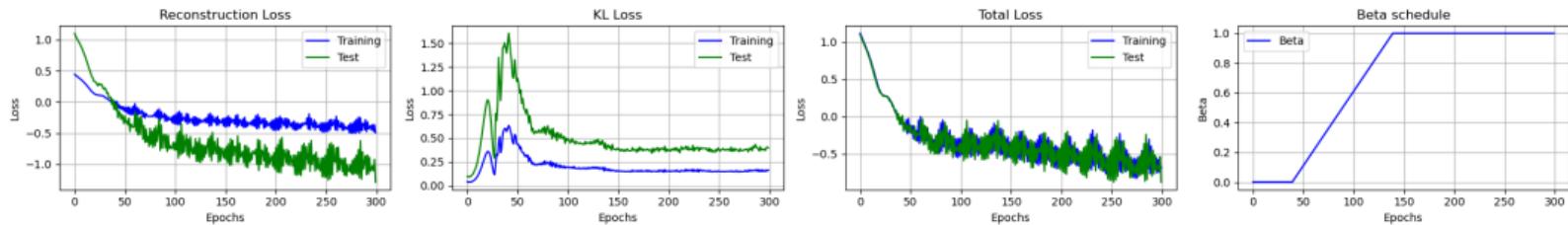
# Code

GitHub repo

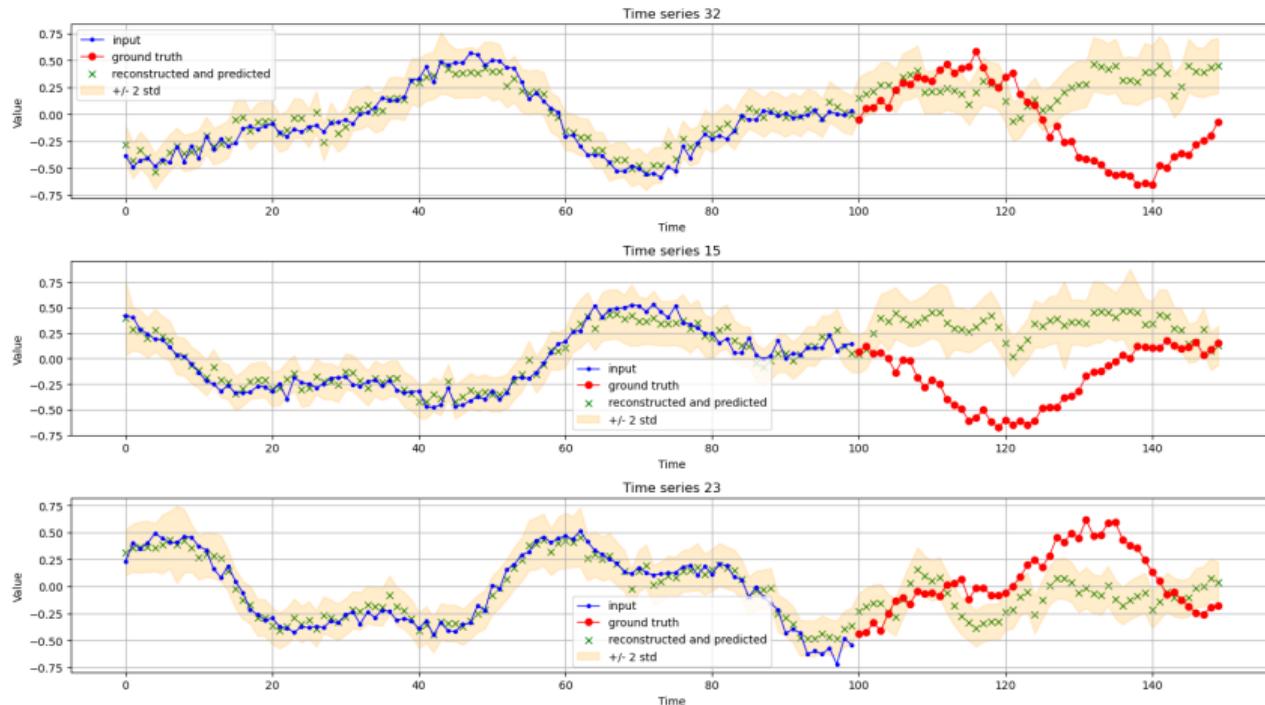
All code at Benjamin GitHub repo

## DKF - Toy training - Loss

- Posterior collapse !
- Need  $\beta$  schedule (weight between reconstruction loss and KL)

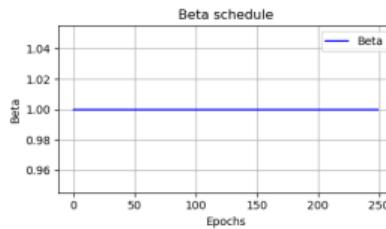
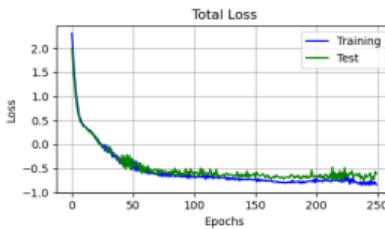
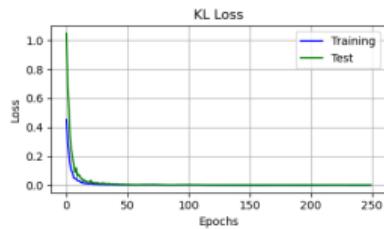
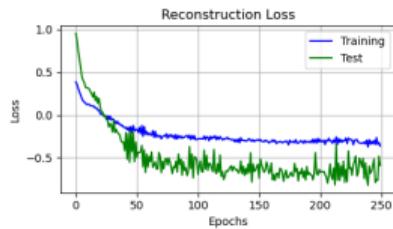


## DKF - Toy training - Generations

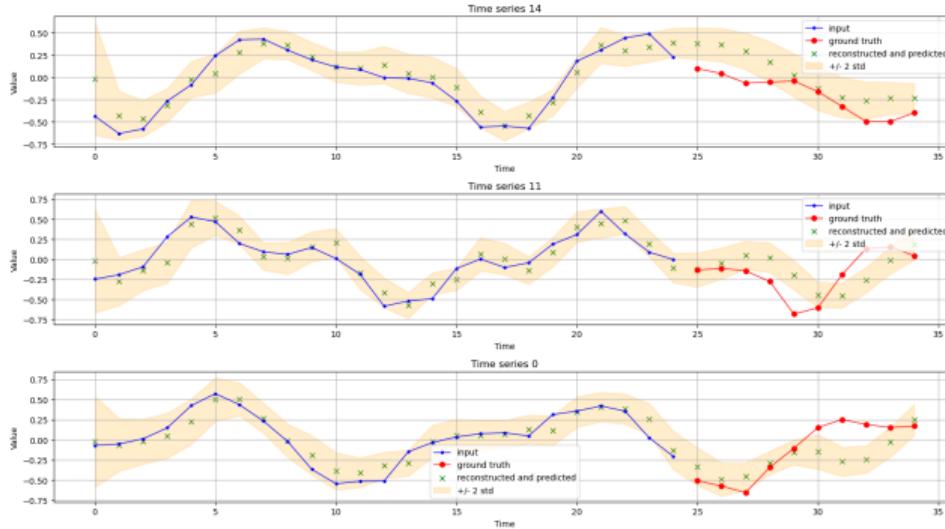


## VRNN - Toy training - Loss

- No posterior collapse
- Shorter toy time series to reduce training time



## VRNN - Toy training - Generation



## Sprites dataset

- Synthetic cartoon characters dataset from [15]
- RGB images  $64 \times 64 \times 3$ .
- Each character has
  - 4 attributes (hair, shoes, top cloth, bottom cloth) with 6 possible values each
  - 3 possible poses (left, front, right)
- Motion across time : 3 possible actions (walk, spell, slash) across 8 consecutive frames.

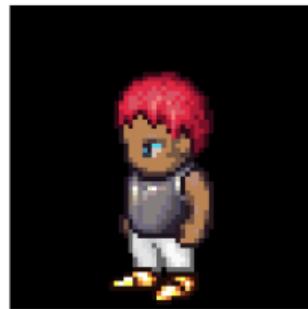
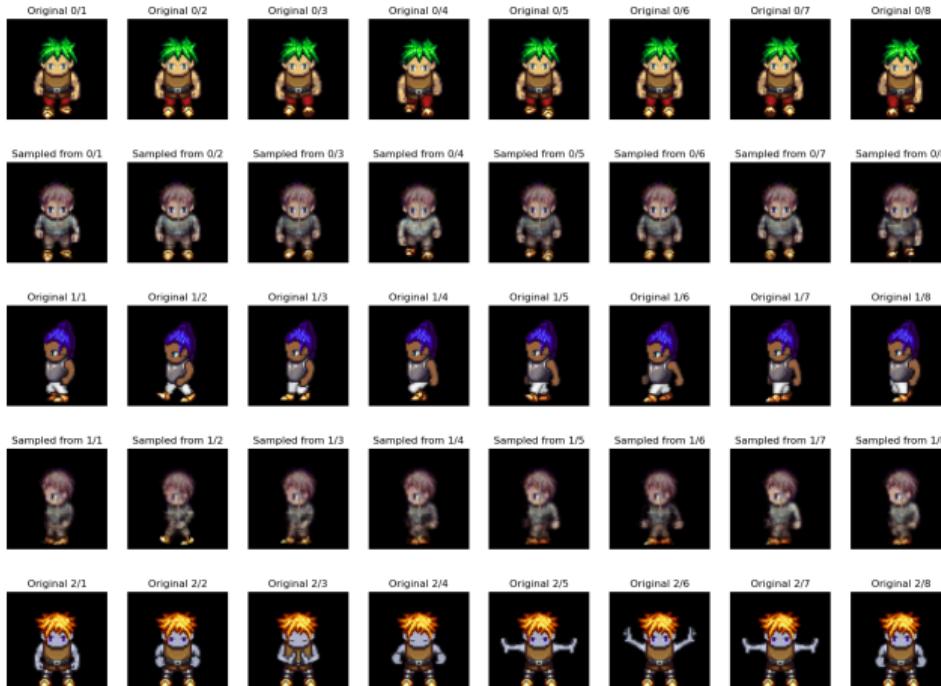


Figure: One sprite

## Sprites series



## VRNN Reconstruction on Sprites



## VRNN Generation

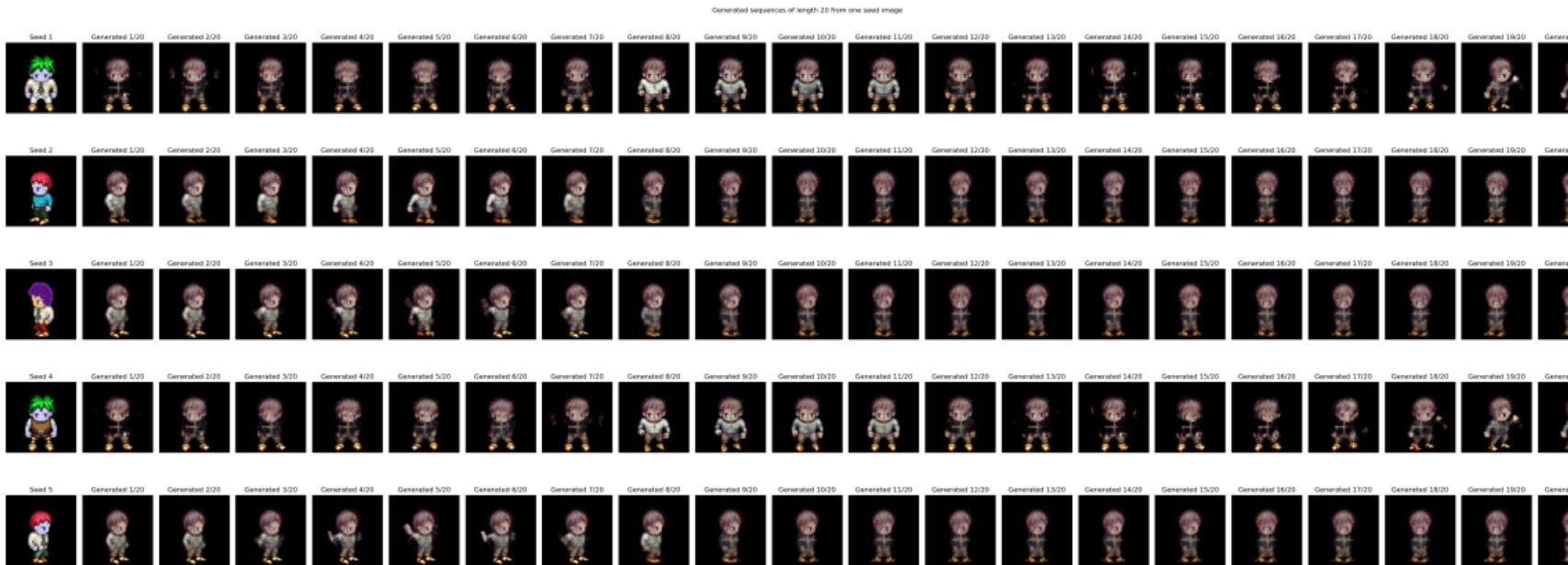
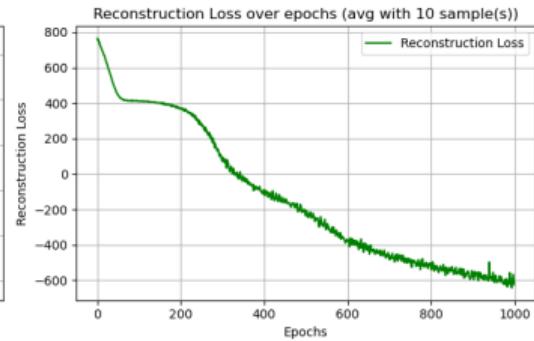
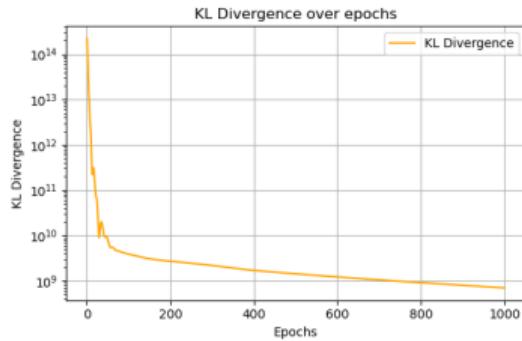
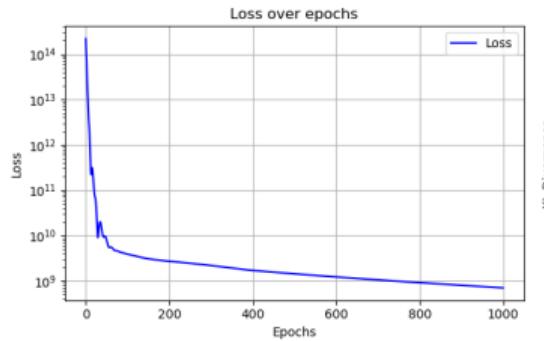


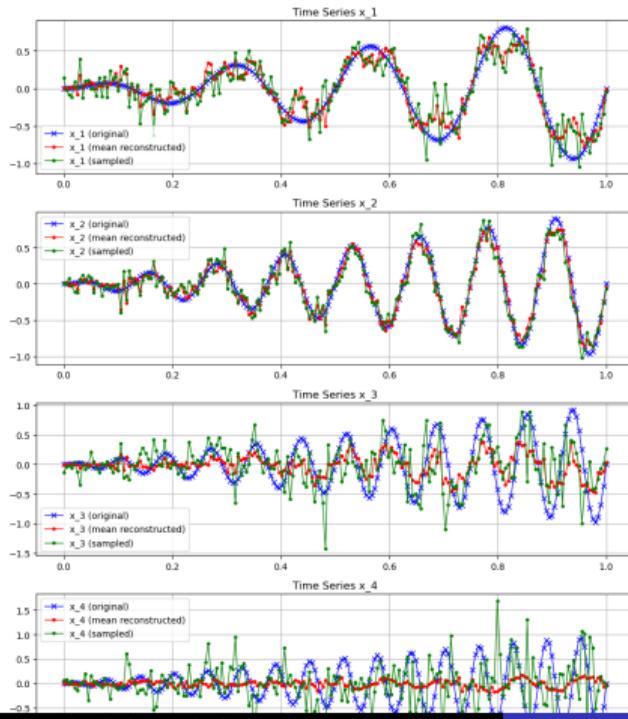
Figure: VRNN Sprites generation

## GPVAE - Toy training - Loss

$D_x = 4$ ,  $D_y = 8$ , RBF kernels with decreasing lengthscales.

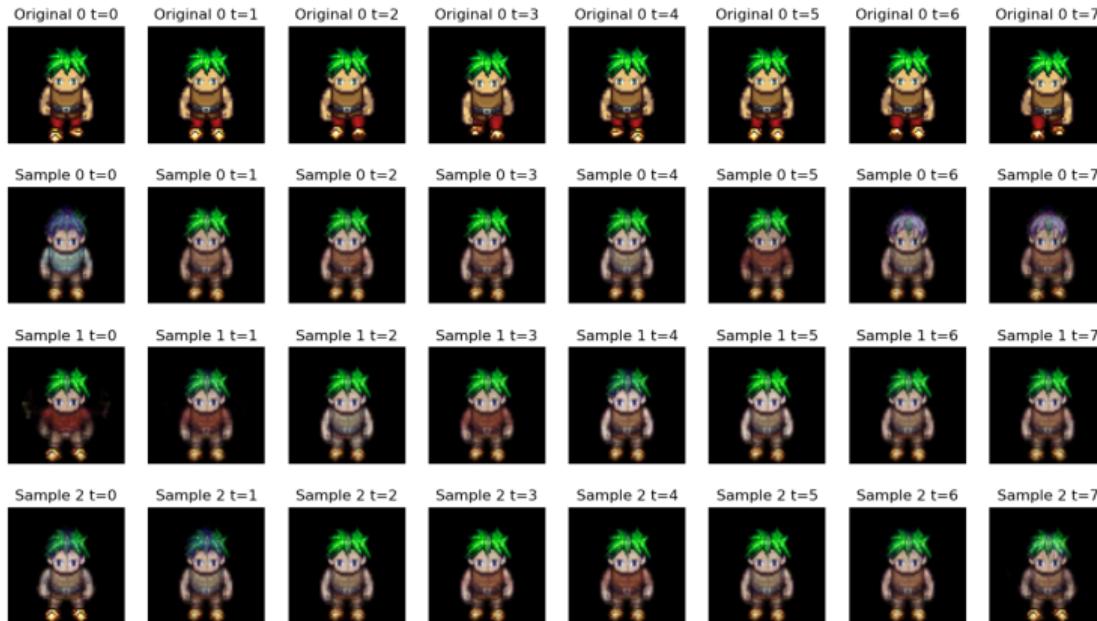


## GPVAE - Toy training - Generations



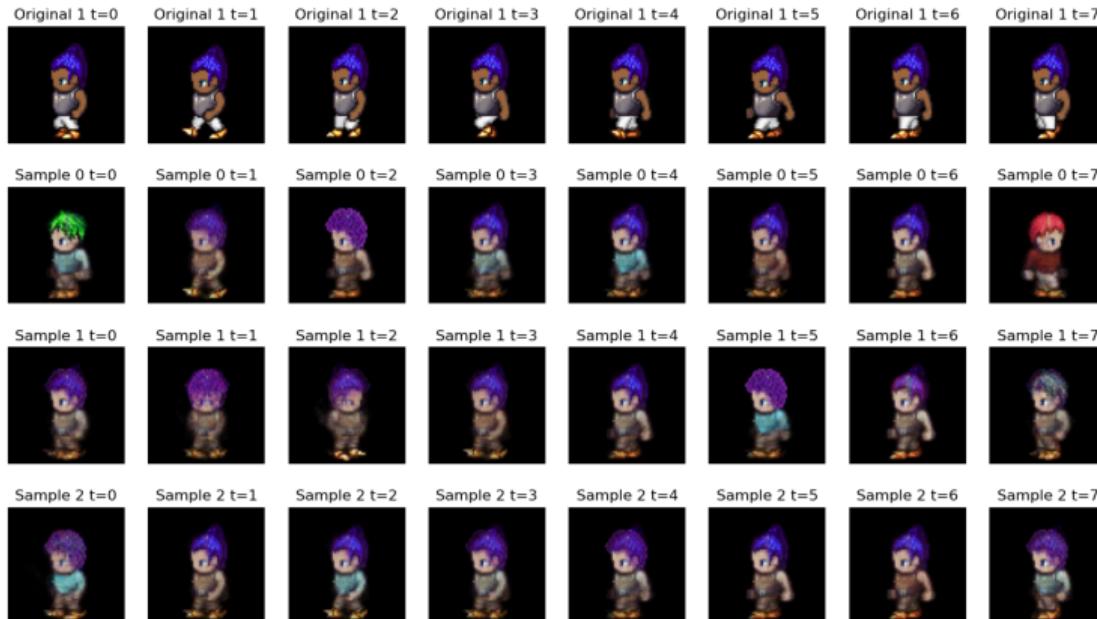
# GPVAE - Sprites Reconstruction - 1

Top: original, below: reconstructions



## GPVAE - Sprites Reconstruction - 2

Top: original, below: reconstructions



# GPVAE - Sprites Reconstruction - 1

Top: original, below: reconstructions



## GPVAE - Generation

Use Gaussian and Matern kernels : not as good as [15] (Cauchy kernels) !!

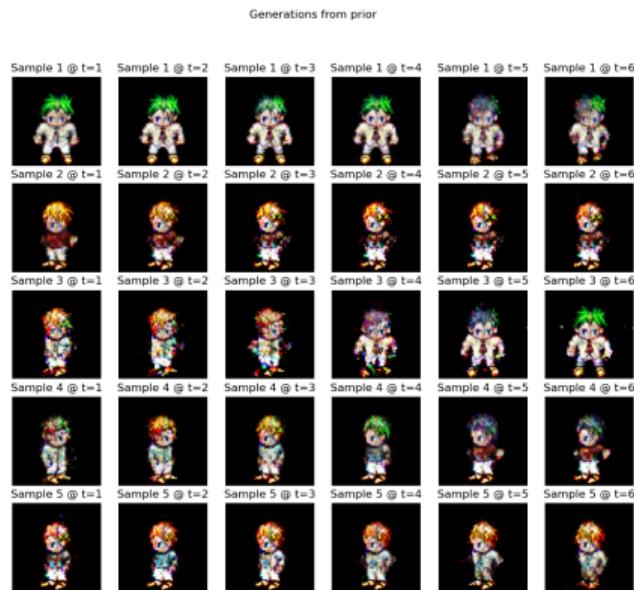


Figure: GPVAE Sprites generation 1

## Stochastic calculus survival kit - Brownian motion

### Definition

A stochastic process  $B = (\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, (B_t)_{t \geq 0}, \mathbb{P})$  with values in  $\mathbb{R}^d$  is called **Brownian motion** iff:

- $B_0 = 0$   $\mathbb{P}$ -a.s.
- $\forall 0 \leq s \leq t$ , the random variable  $B_t - B_s$  is independent from  $\mathcal{F}_s$ .
- $\forall 0 \leq s \leq t$ ,  $B_t - B_s \sim \mathcal{N}(0, Q(t-s))$
- $B$  is continuous <sup>a</sup>

where the matrix  $Q \in \mathbb{S}_d^{++}$  is called the **diffusion matrix**.

---

<sup>a</sup>or more exactly there exists a continuous version of  $B$ , see [16]

A core result is that the quadratic variation of the Brownian motion over an interval  $[s, t]$  (equipped with a subdivision  $\pi = \{s = t_0 < t_1 < \dots < t_k < \dots < t_n = t\}$ ), and defined as the limit when  $|\pi| \rightarrow 0$  of  $V_\pi^{(2)} = \sum_{k=0}^{n-1} |f(t_{k+1}) - f(t_k)|^2$ , is:

$$\lim_{|\pi| \rightarrow 0} V_\pi^{(2)} = Q(t-s) \text{ in } L^2 \quad (42)$$

## Stochastic calculus survival kit - Ito's process

### Definition

A process  $X = (X_t)_{t \in [0, T]}$  is called a **Ito's process** if it can be written as:

$$X_t = X_0 + \int_0^t a_s ds + \int_0^t b_s dB_s \quad \forall t \in [0, T] \tag{43}$$

where  $a$  and  $b$  are two stochastic processes such that the integrals exist (ie  $a \in \Lambda^1$  and  $b \in \Lambda^2$ ). Equivalently, we write  $X_t$  as the solution to the **Stochastic Differential Equation**:

$$dX_t = a_t dt + b_t dB_t$$

## Stochastic calculus survival kit - Ito's formula

### Theorem

*An Itô's process remains an Itô's process when it is transformed by a deterministic function that is "smooth enough".*

*Let  $X$  be a Itô's process on  $[0, T]$  :  $dX_t = a_t dt + b_t dB_t$ .*

*Let  $f : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}, (x, t) \mapsto f(x, t)$  be  $\mathcal{C}^{2,1}$  :  $\mathcal{C}^2$  in  $x$ , and  $\mathcal{C}^1$  in  $t$ .*

*Then  $(f(X_t, t))_{t \in [0, T]}$  is also an Itô's process and:*

$$d(f(X_t, t)) = \frac{\partial f}{\partial t}(X_t, t)dt + \frac{\partial f}{\partial x}(X_t, t)dX_t + \frac{1}{2} \frac{\partial^2 f}{\partial x^2}(X_t, t)b_t^2 dt \quad (44)$$

*The last term is Itô's complementary term.*

*In dimension  $d > 1$ :*

$$d(f(X_t, t)) = \frac{\partial f}{\partial t}(X_t, t)dt + (\nabla f)^T(X_t, t)dX_t + \frac{1}{2} \text{Tr}\left((\nabla \nabla^T f)dX_t dX_t^T\right) \quad (45)$$

# Definition of a Stochastic Differential Equation

## Definition

Let:

- $B$  be a Brownian motion  $B_t \in \mathbb{R}^S$ , of diffusion matrix  $Q$
- $F$  be a deterministic function **drift**  $F : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{D \times D}$
- $L$  be a deterministic function **diffusion** (aka dispersion)  $L : \mathbb{R}^D \times \mathbb{R} \rightarrow \mathbb{R}^{D \times S}$

The SDE is:

$$dX_t = F(X_t, t)dt + L(X_t, t)dB_t \quad (46)$$

$$X_{t_0} = X_0 \quad (47)$$

where  $X_0$  can be a scalar constant or a random variable. A stochastic process  $X$  is said to be solution of 46 if it verifies:

$$\forall t, \quad X_t = X_0 + \int_0^t F(X_u, u)du + \int_0^t L(X_u, u)dB_u$$

## A solution to an SDE is a Markov Process

- As for Ordinary Differential Equation (ODE), a solution to 46 might not exist. Also, results similar to Cauchy-Lipschitz exist for existence and unicity, based on assumptions on  $F$  and  $L$ .
- Intuitively, we can see that an "infinitesimal increment" of  $X_t$  to  $X_{t+\Delta t}$  verifies :  
 $\Delta X_t \approx F(X_t, t)\Delta t + L(X_t, t)dB_t$ . But  $dB_t$  is a Brownian increment independent of  $X_t$ , This suggests that  $X_{t+\Delta t}$  depends on the past only by  $X_t$ .
- In other words,  $X_t|\mathcal{F}_s = X_t|X_s$  for any  $0 < s < t$ . ie : **the solution of a SDE is a Markov process.** (The formal proof is given in [16].)

The solution to a SDE is a Markov process

# Linear SDE

A particularly useful flavor of SDE is the linear SDE, that allows some close-form (or at least nicer) solutions:

## Definition

With the same notations as 46:

The linear SDE is:

$$dX_t = F(t)X_t dt + L(t)dB_t \quad (48)$$

$$X_{t_0} = X_0 \sim \mathcal{N}(m_0, P_0) \quad (49)$$

## Transition kernels for linear SDEs

In this case, the transition kernels family and the solution write:

$$\Psi : \mathbb{R}^2 \rightarrow \mathbb{R}^D \quad (50)$$

$$\frac{\partial \Psi(\tau, t)}{\partial \tau} = F(\tau)\Psi(\tau, t) \quad (51)$$

$$\frac{\partial \Psi(\tau, t)}{\partial t} = -\Psi(\tau, t)F(t) \quad (52)$$

$$\Psi(\tau, t) = \Psi(\tau, s)\Psi(s, t) \quad (\text{Chapman-Kolmogorov}) \quad (53)$$

$$\Psi(\tau, t) = \Psi(t, \tau)^{-1} \quad (54)$$

$$\Psi(t, t) = I_d \quad (55)$$

$$X_t = \Psi(t, t_0)X_0 + \int_{t_0}^t \Psi(t, \tau)L(\tau)dB_\tau \quad (56)$$

$$X_{t_0} = X_0 \sim \mathcal{N}(m_0, P_0) \quad (57)$$

The solution to a Linear SDE is a Gaussian process. (The converse is NOT true!)

## General Filtering/Smoothing equations with SDEs

- In practice, we posit a stochastic process prior defined by a general SDE, and we have discrete-time measurements.
- Formally, the Continuous-Discrete State Space Model (CD-SSM) is defined by:

### Continuous-Discrete State Space model

$$dZ_t = F(Z_t, t)dt + L(Z_t, t)dB_t \quad (58)$$

$$x_k \sim p(x_k | z_{t_k}) \quad (59)$$

where:

- $Z_t \in \mathbb{R}^D$  is the *state*, ie a stochastic process defining the latent variable.
- $B_t \in \mathbb{R}^S$  is a Brownian motion with diffusion matrix  $Q$ .
- $F \in \mathbb{R}^D$  and  $L \in \mathbb{R}^{D \times S}$  are the usual drift and dispersion functions.
- $x_k$  are the observations taken at **discrete times**  $(t_k)_{k=1, \dots, n}$

NB : the observations are assumed to conditionnally independent of the state.

# Filtering

- **Filtering** is the problem of determining the posterior probability of the latent  $Z_t$  given the discrete measurements, ie finding  $p(Z_t|x_{1:k})$  with  $t_k \leq t$ . This corresponds to determining the generative transition probability  $p_{\theta_z}(z_t|z_{1:t-1}, x_{1:t-1})$  in our DVAE setting.
- In general, close-form solutions can be derived when the latent variables SDE is linear. In continuous time, we get the **Kalman-Bucy** filter equations, which discretize in the well-known **Kalman filter**.

# Filtering

## Kalman-Bucy filter

$$dZ_t = F(t)Z_t dt + L(t)dB_t \quad (60)$$

$$dX_t = H(t)X_t dt + d\eta_t \quad (61)$$

NB : the observations are assumed to conditionnally independent of the state. Then the Bayesian filter (Kalman-Bucy) is:

$$p(z_t | x_{<t}) = \mathcal{N}(Z_t | m_t, P_t) \quad (62)$$

$$K = PH(t)^T R^{-1} \quad (63)$$

$$dm = F(t)mdt + K(dX_t - H(t)mdt) \quad (64)$$

$$\frac{dP}{dt} = F(t)P + PF(t)^T + L(t)QL(t)^T - KRK^T \quad (65)$$

# Smoothing

- **Smoothing** is the problem of determining the posterior probability of the latent  $Z_t$  given all known observations, ie finding  $p(Z_t|x_{1:T})$  for all  $t \in [0, T]$ .
- This corresponds to determining the inference model  $q_\phi(z_t|z_{1:t-1}, x_{1:T})$  in the DVAE setting.
- Discretizing the transition density in CD-SSM, we have

$$Z_{t_{k+1}} \sim p(Z_{t_{k+1}}|Z_{t_k}) \tag{66}$$

$$X_k \sim p(X_k|Z_{t_k}) \tag{67}$$

## GP-VAE with accomodating kernels : filtering/smoothing in $O(n)$

- We wrap up here linking the filtering/smoothing theory of linear SDE with the GP-VAE model of [8].
- Using the formalization above, a GP-VAE with Gaussian observation is basically:

$$Z_t \sim \mathcal{GP}(m(\bullet), k(\bullet, \bullet)) \quad (68)$$

$$X_{t_k} \sim \mathcal{N}(X_{t_k} | Z_{t_k}, \sigma^2) \quad (69)$$

- Computing the posterior distribution  $p(Z_t | X_{t_1:t_T})$  is performing a Gaussian Process regression (see [22]), which naively scales in  $O(n^3)$ .
- However, if the Gaussian process can be written as a linear SDE:

$$dZ_t = F(t)Z_t dt + L(t)dB_t \quad (70)$$

$$X_{t_k} \sim \mathcal{N}(X_{t_k} | Z_{t_k}, \sigma^2) \quad (71)$$

then the Kalman filter and smoother apply, that scale in  $O(n)$ .

### GP Prior regression in $O(N)$ cost

If the GP prior can be written as the solution to a linear SDE, then the GP prior regression problem can be performed with linear cost with the Kalman-Bucy equations.

## Latent ODE

- Latent ODEs is a class of models introduced in [3] : "Neural Ordinary Differential Equations" by Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, David Duvenaud. ArXiV : Neural ODE Best Paper Award NeurIPS 2018.
- Starting point : assume ResNet-like evolution of latent

$$z_{t+1} = z_t + f(z_t, \theta_t) \quad (72)$$

- becomes in continuous time:

$$\frac{dz_t}{dt} = f(z_t, t, \theta_f) \quad (73)$$

where  $\theta_f$  is a set of parameters, that can typically be the parameters of a neural network learning  $f$ .

## Latent ODE - model

- Generative model

$$z_{t_0} \sim p_{\theta_z}(z_{t_0}) \quad (74)$$

$$z_{t_1}, z_{t_2}, \dots, z_{t_N} = \text{ODE Solver}(z_{t_0}, f, \theta_f, t_0, \dots, t_N) \quad (75)$$

$$x_{t_i} \sim p_{\theta_x}(x_t | z_t) \quad (76)$$

- Inference

$$[\mu_\phi, \Sigma_\phi] = \text{LSTM}(x_{t_0:t_N}) \quad (77)$$

$$q_\phi(z_{t_0} | x_{t_0:t_N}) = \mathcal{N}(z_{t_0} | \mu_\phi, \Sigma_\phi) \quad (78)$$

## Latent ODE - model

We reproduce here the drawing from the paper:

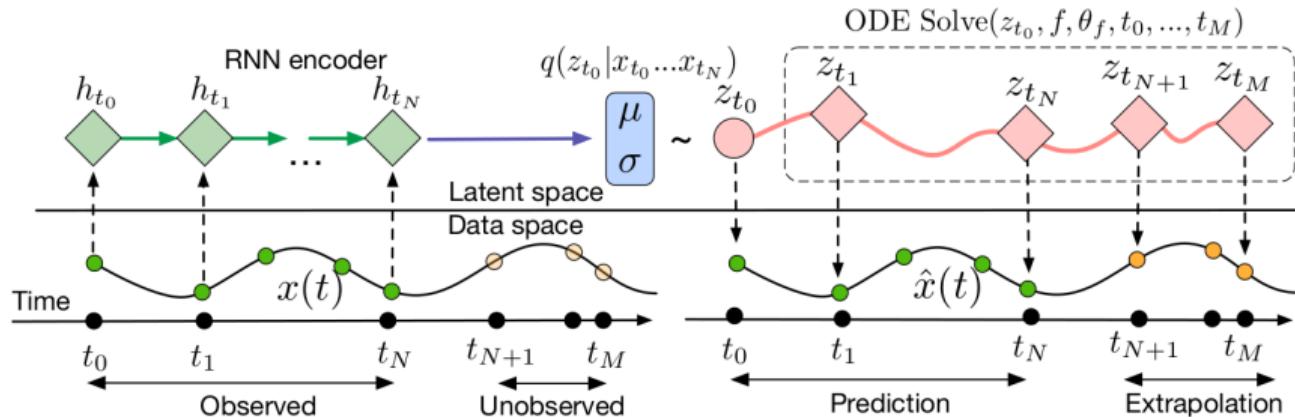


Figure: Neural ODE model

## Latent ODE - ELBO

- the stochastic variables are  $z_{t_0}$  and the  $x_{t_i}$ 's.
- the joint distribution writes:

$$p(x_{t_1:t_N}, z_{t_0}) = p(z_{t_0}) \prod_{t=1}^N p_{\theta_x}(x_{t_i} | z_{t_i}) \quad (79)$$

- likelihood:

$$\log p(x_{t_1:t_N}) \geq \mathbb{E}_{q_\phi(z_{t_0} | x_{t_1:t_N})} \log \frac{p(x_{t_1:t_N}, z_{t_0})}{q_\phi(z_{t_0} | x_{t_1:t_N})} \quad (80)$$

$$= \sum_{i=1}^N \mathbb{E}_{q_\phi(z_{t_0} | x_{t_1:t_N})} \log p_{\theta_x}(x_{t_i} | z_{t_i}) - \mathbb{KL}(q_\phi(z_{t_0} | x_{t_1:t_N}) || p(z_{t_0})) \quad (81)$$

- Need to compute the gradients of  $\log p_{\theta_x}(x_{t_i} | z_{t_i})$  w.r.t.  $\theta_f$ . Methods are forward sensitivity, backpropagation through ODE solver, or **adjoint sensitivity method**. (see [21], [26]).

## Latent SDE Model

Latent ODEs models have limitations :

- the latent dynamic is deterministic by design
- the initial variable  $z_{t_0}$  encompasses the entire randomness of the prior, and can become unnaturally large to account for randomness along the entire timeline

The idea in [14] is to add some noise to the deterministic computation of the latent variable:

$$\frac{dz_t}{dt} = f_{\theta_f}(z_t, t) + \epsilon_t \quad (82)$$

$$\epsilon_t \sim \mathcal{N}(0, QId) \quad (83)$$

Which leads to an SDE prior:

$$dZ_t = f_{\theta}(Z_t, t)dt + \sigma_{\theta}(Z_t, t)dB_t \quad (84)$$

$$Z_{t_0} \sim Z_0 \quad (85)$$

(where we used  $\sigma_{\theta}$  instead of our usual  $L(Z_t, t)$  to stick to the notations of the paper).

84 defines a prior distribution over functions. In order to draw a sample function, we would:

- draw a sample  $z_{t_0} \sim Z_0$
- draw a random Brownian motion  $\tilde{B}_t$  path from  $B_t$
- compute  $z_t - z_{t_0} = \int_{t_0}^t f_{\theta}(Z_t, t)dt + \int_{t_0}^t \sigma_{\theta}(Z_t, t)d\tilde{B}_t$

## Latent SDE - generative model

The approximate posterior can also be described as a SDE:

$$dZ_t = f_\phi(Z_t, t)dt + \sigma_{\phi=\theta}(Z_t, t)dB_t \quad (86)$$

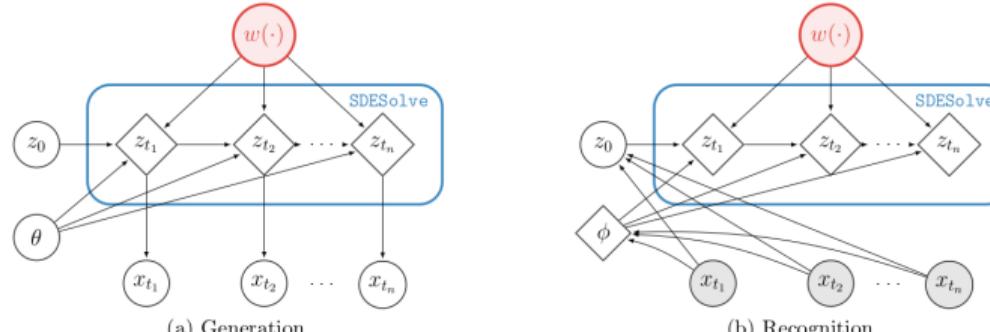
$$Z_{t_0} = z_0 \text{ from prior} \quad (87)$$

- the prior and the approximate posterior share the same diffusion for the KL to have the same support
- the prior and the approximate posterior have the same starting value  $z_0$

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## Latent SDE - inference

- neural networks to learn the drift  $f_\phi$  and the diffusion  $\sigma_\theta$
- requires to compute the gradient of functionals (loss) of type:

$$L(\theta, \phi) = L \left( \int_{t_0}^{t_1} f_\phi(Z_t, t) dt + \int_{t_0}^t \sigma_\theta(Z_t, t) dB_t \right) \quad (88)$$

where  $\int_{t_0}^t \sigma_\theta(Z_t, t) dB_t$  is actually a random variable!

- It appears that the adjoint sensitivity method can be adapted to SDEs (see [14]).

The stochastic VLB writes:

$$\mathcal{L}(\theta, \phi, x_{1:T}) = \mathbb{E} \left( \frac{1}{2} \int_0^T \left| \frac{f_\theta(z_t, t) - f_\phi(z_t, t)}{\sigma_\theta(z_t, t)} \right|^2 dt - \sum_{i=1}^N \log p_{\theta_x}(x_{t_i} | z_{t_i}) \right) \quad (89)$$

## Take-aways

- DVAEs are a natural and powerful extension of VAEs in which the prior expresses the temporal dependency of the data sequence.
- Discrete-time DVAEs use discretized latent priors to encode temporal dynamics. They work best with regularly spaced data.
- Continuous-time DVAEs posit a stochastic process as prior for the latent variables. This allows additional flexibility and irregularly-sampled data.
- In GP-VAE, the latent prior is a Gaussian Process that can sometimes be expressed as a solution to a linear SDE. In that case, Kalman-Bucy filtering and smoothing algorithms can speed up computations.
- Stochastic calculus provides a framework for more general continuous-time priors.
- When expressed as solutions to general SDE, those more general stochastic process priors are used in Latent SDEs.

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# Thank you for your attention!

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# Glossary I

**CD-SSM** Continuous-Discrete State Space Model. 56, 59

**DAG** Directed Acyclic Graph. 18

**DKF** Deep Kalman Filter. 3–6

**DVAE** Dynamical Variational Auto Encoder. 3–6, 19, 25, 57, 59, 68–73

**ELBO** Evidence Lower Bound. 21

**GP** Gaussian Process. 3–6, 29, 31, 60

**GP-VAE** Gaussian Process Variational Auto Encoder. 3–6, 60, 68–73

**GPM** Graphical Probabilistic Model. 7, 8, 10–13, 25

**Latent ODE** Latent Ordinary Differential Equation model. 3–6, 61, 65

**Latent SDE** Latent Stochastic Differential Equation model. 3–6, 68–73

**LSTM** Long Short Term Memory. 23, 27

## Glossary II

**MLP** Multi Layer Perceptron. 23

**ODE** Ordinary Differential Equation. 53, 64

**SDE** Stochastic Differential Equation. 3–6, 52–57, 60, 65, 66, 68–73

**SSM** State Space Model. 18

**VAE** Variational Auto Encoder. 3–6, 68–73

**VLB** Variational Lower Bound. 7, 8, 22, 25, 26, 67

**VRNN** Variational Recurrent Neural Network. 3–6, 25