

Dynamical Variational Autoencoders Links to stochastic differential equations

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Summary

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2 Dynamical Variational AutoEncoders - Theory

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Abstract

- **Variational Auto Encoders (VAEs)** have limitations when dealing with data sequences.
- **Dynamical Variational Auto Encoders ([10])** are adapted to data sequences
 - Temporal dependency built into latent generative model
 - Discrete or continuous time prior models
 - 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 Neural Stochastic Differential Equations (Neural-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 Neural Ordinary Differential Equations (Neural-ODEs) and Neural-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. $u_{t_i}, i = 1, \dots, T$)
- Prior encoding a temporal dependency over z_t
- 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 maximize 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 $q_\phi(z_{1:T}|x_{1:T})$ (ϕ 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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- Good practice : use the true posterior expression $p(z_{1:T}|x_{1:T})$ for $q_\phi(z_t|z_{1:t-1}, x_{1:T})$

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

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

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

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

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

Likelihood

- Observation model and encoder:

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

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

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 with neural nets.

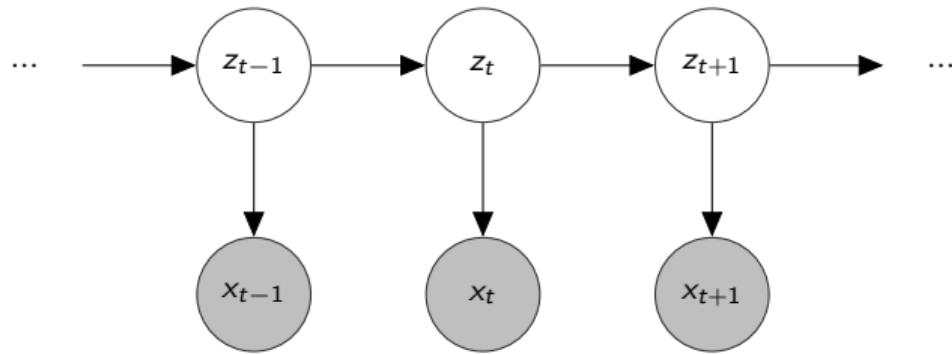


Figure: Probabilistic model of a Deep Kalman Filter

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_{θ_x} , p_{θ_z} and q_ϕ (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

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

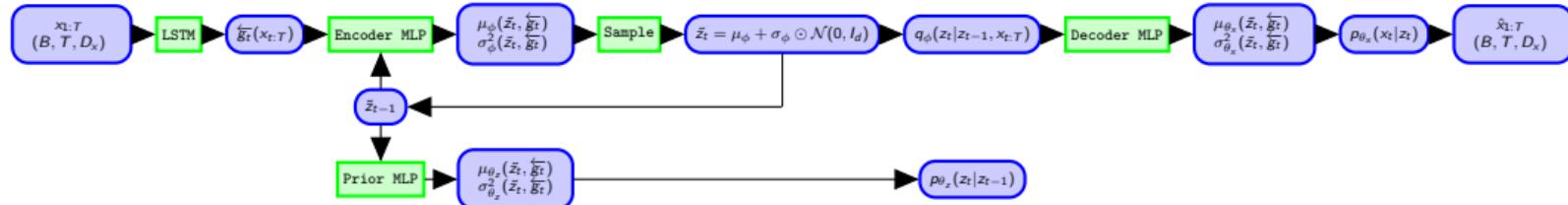
DKF - Torch

- 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:



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

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, to account for the full unsimplified expressions. Specifically:

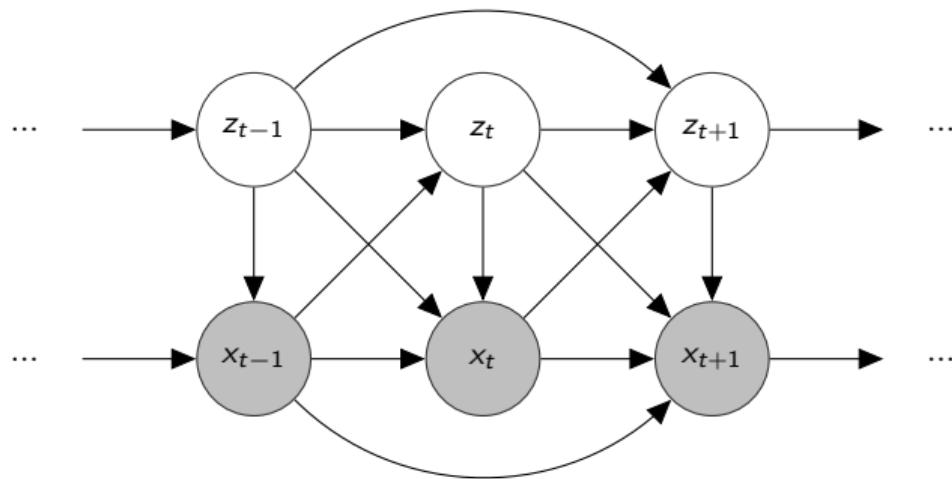


Figure: Probabilistic model of a Variational RNN

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**

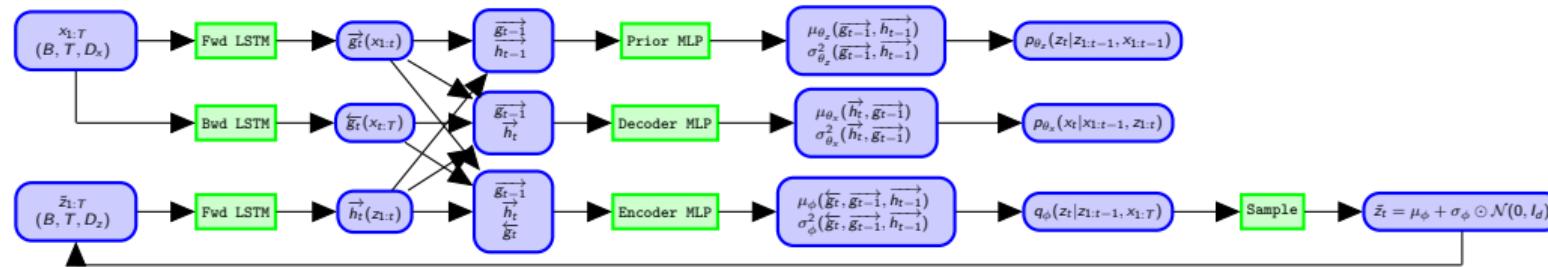
$$q_{\phi}(z_t | z_{1:t-1}, x_{1:T}) = \mathcal{N}(z_t | \mu_{\phi}(z_{1:t-1}, x_{1:T}), \text{diag } \sigma_{\phi}^2(z_{1:t-1}, x_{1:T})) \quad (28)$$

- **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.



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

Gaussian Process - Variational Auto Encoder

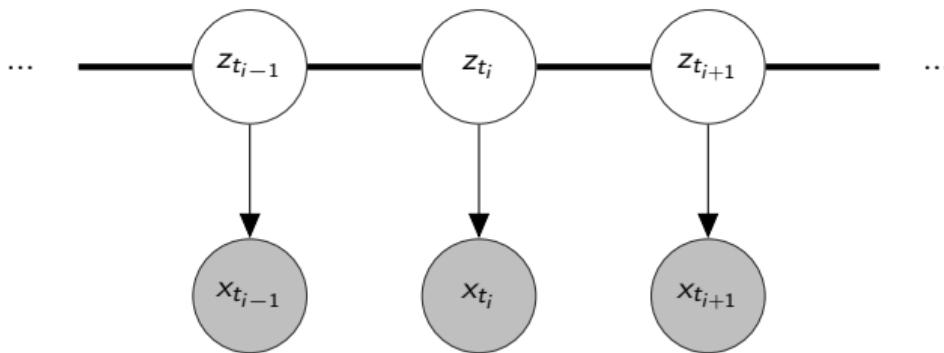


Figure: Probabilistic model of a GP-VAE

- **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_{θ_x}

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

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

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

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

Can code covariance with covariance matrix Σ_ϕ^l , precision matrix Λ_ϕ^l , or with a Cholesky decomposition $L_\phi^l L_\phi^l$.

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 .
 - 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

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

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

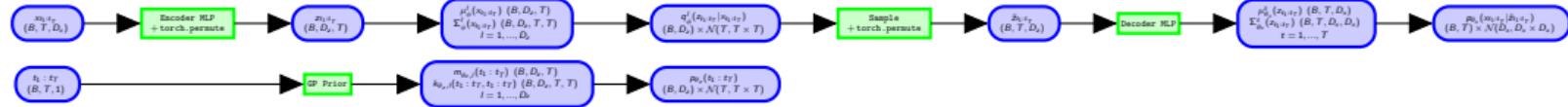
$$q_\phi(z_{t_1:t_T}^l | x_{t_1:t_T}^l) = \mathcal{N}(m_\phi^l(x_{t_1:t_T}), \Sigma_\phi^l(x_{t_1:t_T})) \quad l = 1, \dots, L \quad (38)$$

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

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

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

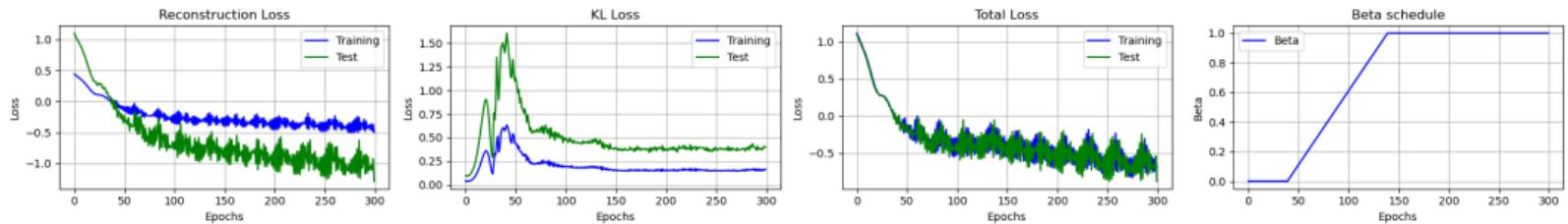
GP-VAE - Torch



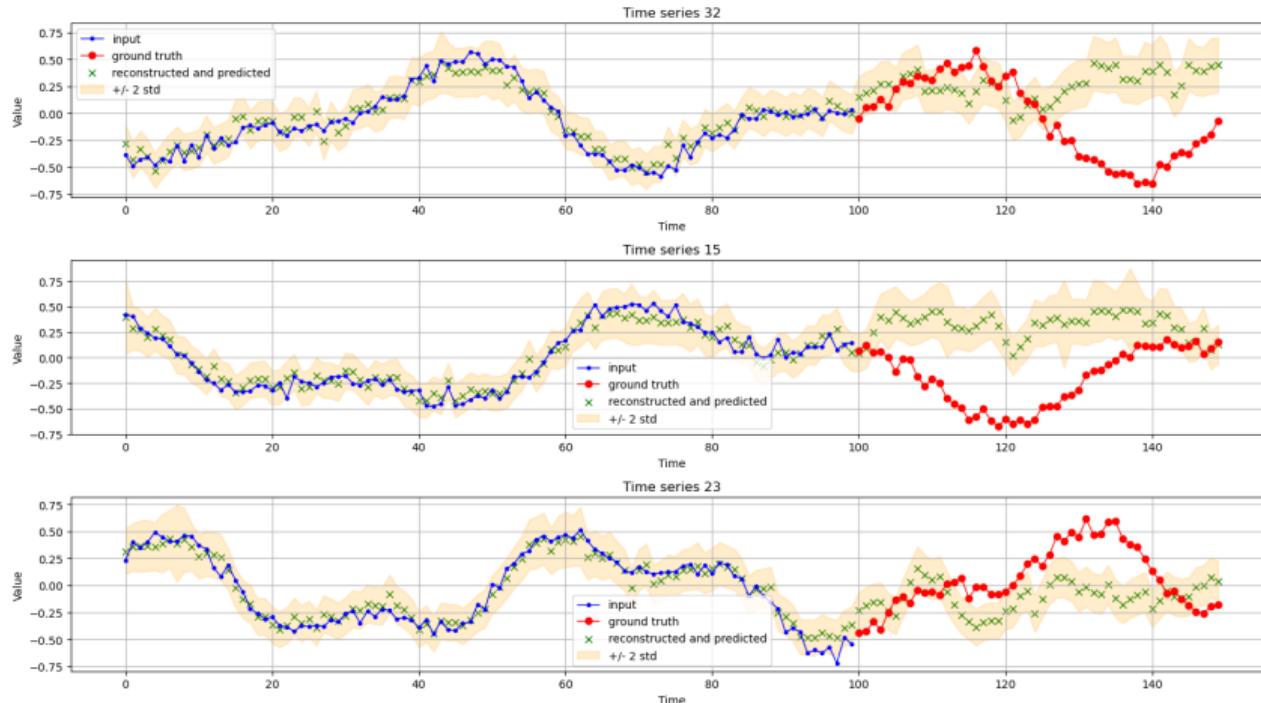
$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^T \mathbb{E}_{q_\phi(z_{t_i} | x_{t_1:t_T})} \log p_{\theta_x}(x_{t_i} | z_{t_i}) - \mathbb{KL}(q_\phi(z_{t_1:t_T} | x_{t_1:t_T}) || p_{\theta_z}(z_{t_1:t_T}))$$

DKF - Toy training - Loss

- Posterior collapse !
- Need β schedule (weight between reconstruction loss and KL)

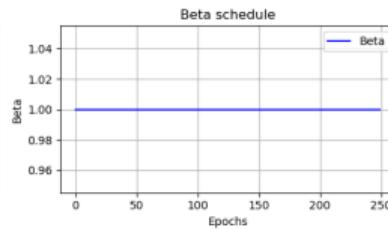
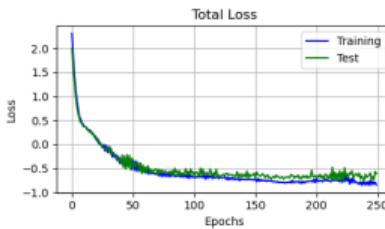
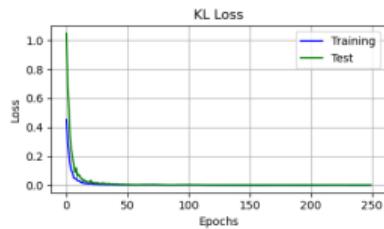
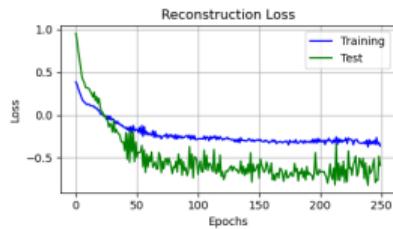


DKF - Toy training - Generations

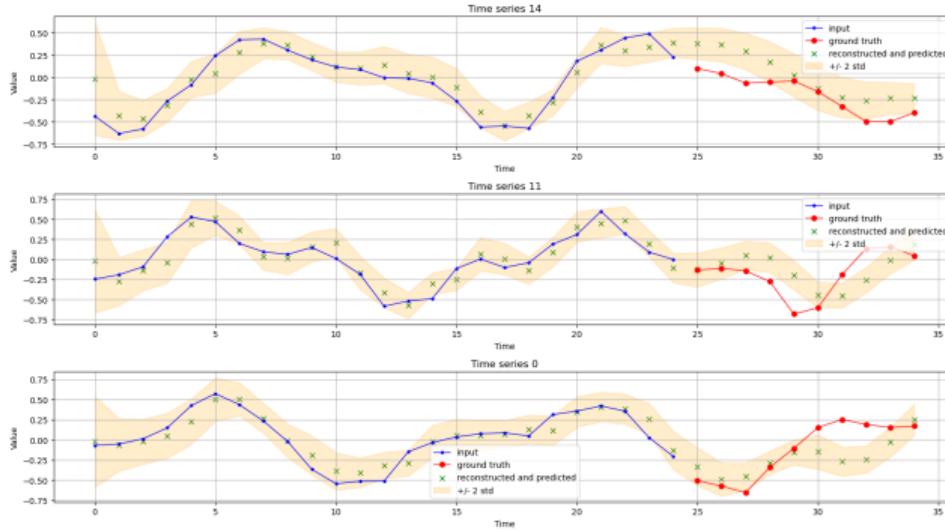


VRNN - Toy training - Loss

- 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.

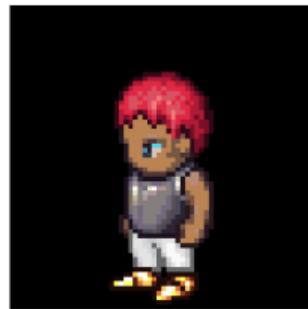
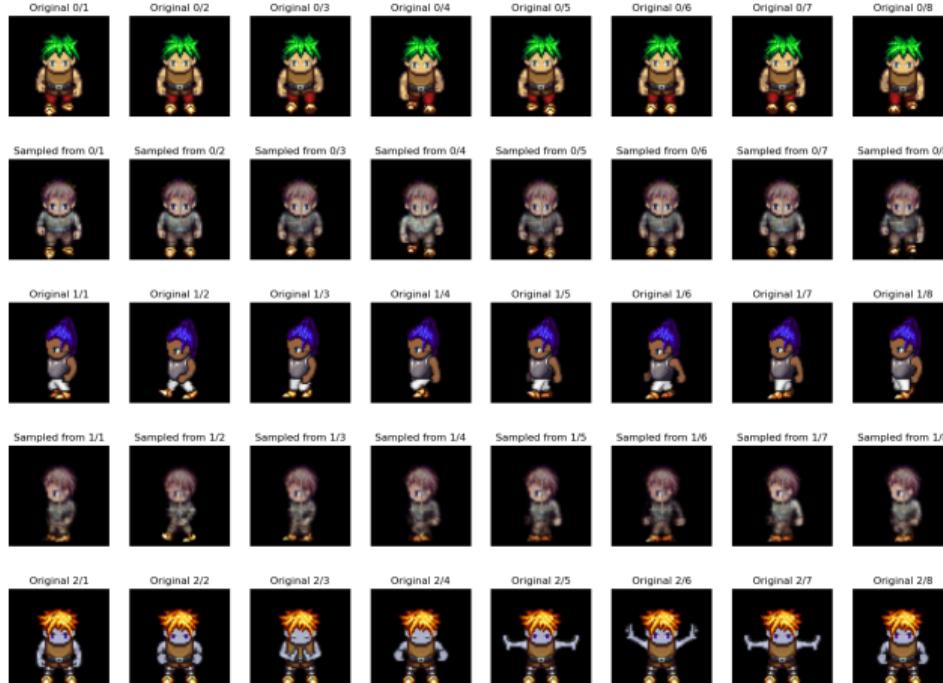


Figure: One sprite

Sprites series



VRNN Reconstruction on Sprites



VRNN Generation

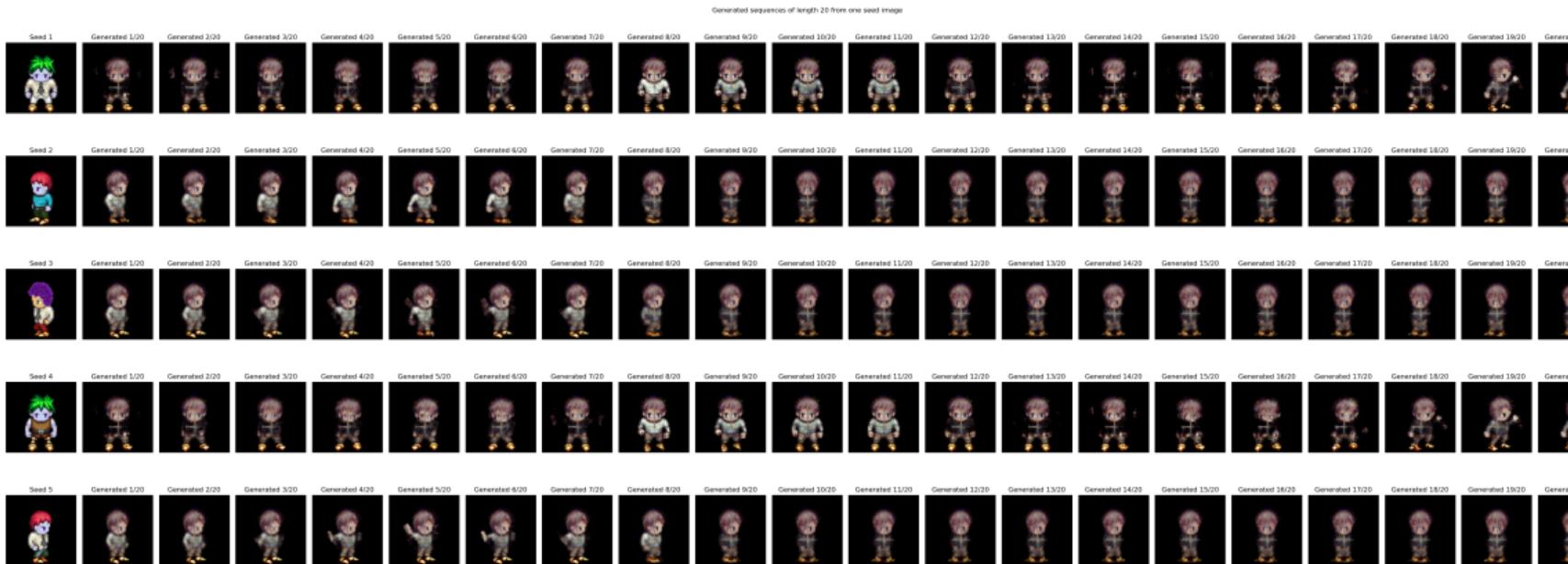
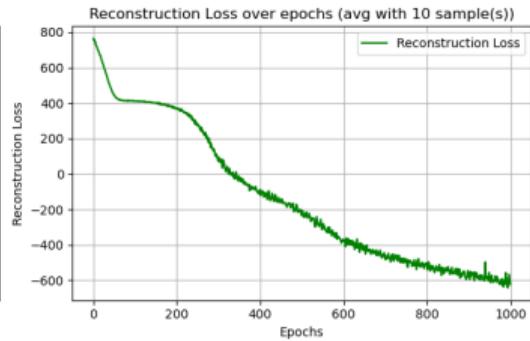
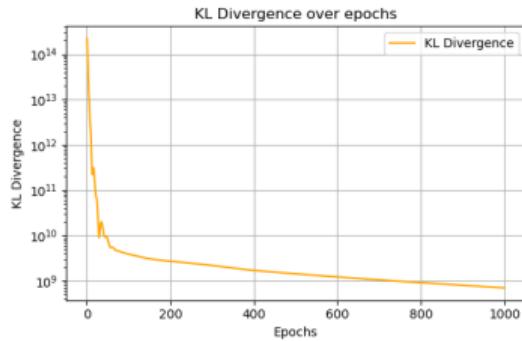
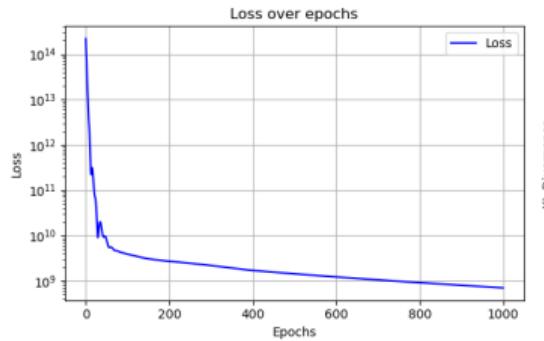


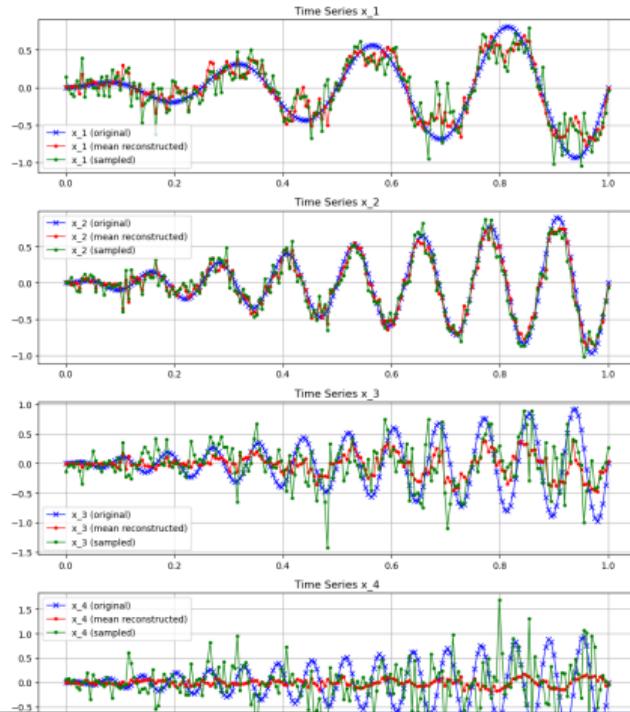
Figure: VRNN Sprites generation

GPVAE - Toy training - Loss

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

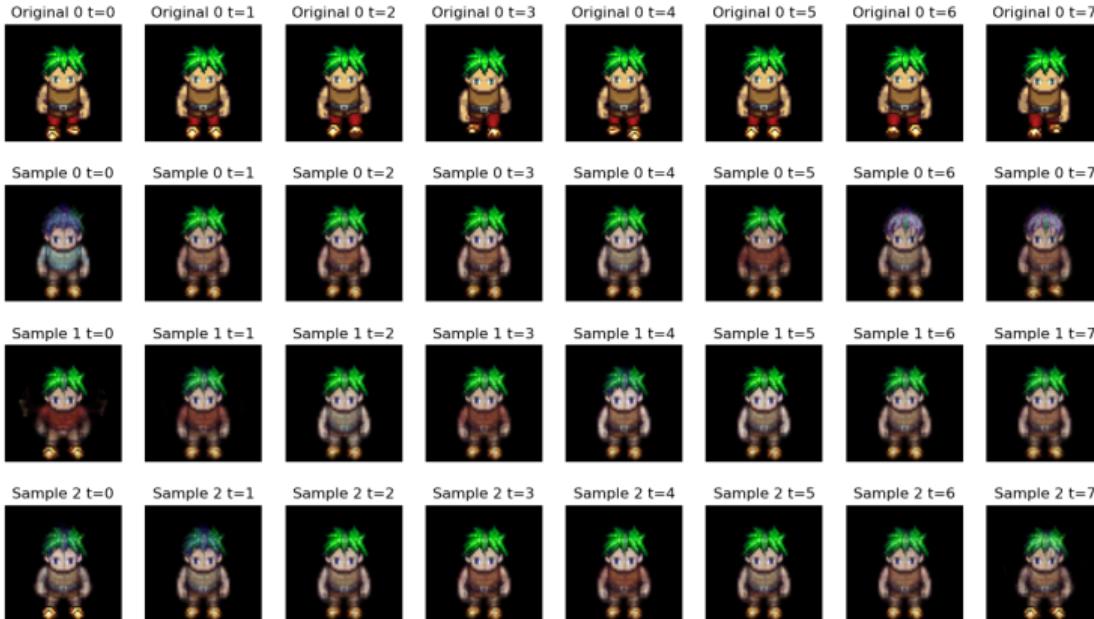


GPVAE - Toy training - Generations



GPVAE - Sprites Reconstruction - 1

Top: original, below: reconstructions



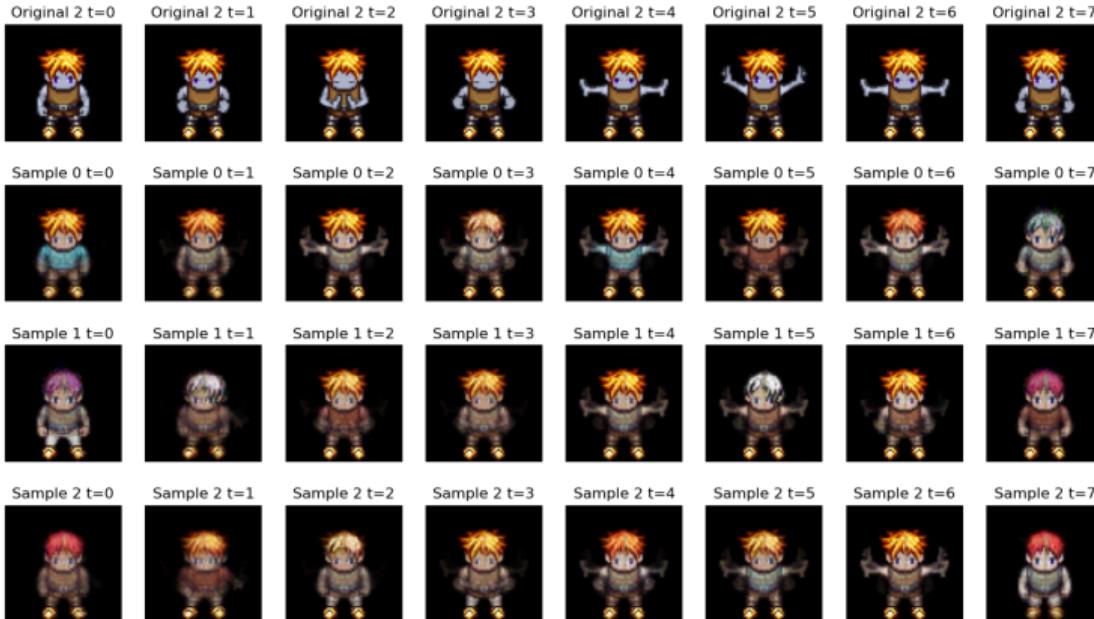
GPVAE - Sprites Reconstruction - 2

Top: original, below: reconstructions



GPVAE - Sprites Reconstruction - 1

Top: original, below: reconstructions



GPVAE - Generation

Generations from prior



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}_t .
- $\forall 0 \leq s \leq t$, $B_t - B_s \sim \mathcal{N}(0, Q(t-s))$
- B is continuous ^a

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

^aor 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:

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

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

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

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

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

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

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

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

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.

Neural ODE

- Neural-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 θ_f is a set of parameters, that can typically be the parameters of a neural network learning f .

Neural 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

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

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

Neural ODE - model

We reproduce here the drawing from the paper:

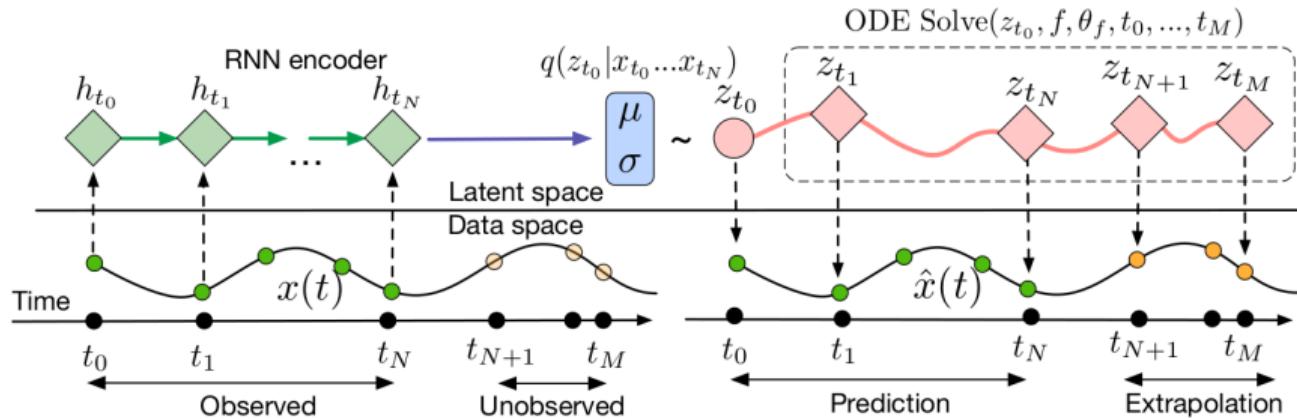


Figure: Neural ODE model

Neural ODE - ELBO

- the stochastic variables are z_{t_0} and the x_{t_i}
- 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. θ_f . Methods are forward sensitivity, backpropagation through ODE solver, or **adjoint sensitivity method**. (see [21], [26]).

Neural SDE

Neural SDE

Outro

It's been quite a personal journey...

Wrapping up:

- DVAEs are a powerful evolution of VAEs where the structure of the set of latent variables aims at expressing the temporal dependencies.
- Discrete-time DVAEs give structure to latent variables 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.
- **The specific model GP-VAE, where the latent prior is a Gaussian Process can be expressed as a solution to a linear SDE, can use well-known linear-time filtering and smoothing algorithms to speed up computations.**
- Stochastic calculus provides a framework for continuous-time priors.
- More general stochastic process priors can be used, expressed as solutions to general SDE : those are latent SDE models.

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CD-SSM Continuous-Discrete State Space Model. 54, 57

DAG Directed Acyclic Graph. 18

DKF Deep Kalman Filter. 3–6

DVAE Dynamical Variational Auto Encoder. 3–6, 19, 25, 55, 57, 64

ELBO Evidence Lower Bound. 21

GP Gaussian Process. 3–6, 29, 30, 58

GP-VAE Gaussian Process Variational Auto Encoder. 3–6, 58, 64

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

LSTM Long Short Term Memory. 23, 27

MLP Multi Layer Perceptron. 23

Neural-ODE Neural Ordinary Differential Equation. 3–6, 59

Neural-SDE Neural Stochastic Differential Equation. 3–6

ODE Ordinary Differential Equation. 51, 62

SDE Stochastic Differential Equation. 3–6, 50–55, 58, 64

SSM State Space Model. 18