Dynamical Variational Autoencoders
Links to stochastic differential equations

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Summary

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 $t_1, t_2, ...t_T$ or irregular $t_{i_1}, t_{i_2}, ..., t_{i_T}$ sampling times
- Observations : a sequence of T points $x_{1:T} = \{(x_t)_{t=1,...,T}\}$ (or $x_{t_{i_1}:t_{i_T}} = \{(x_{t_i})_{i=1,...,T}\}$) $\in \mathbb{R}^F$.
- Latent variables : an associated sequence of T latent variables $z_{1:T} = \{(z_t)_{t=1,...,T}\} \in \mathbb{R}^L$ (resp. $z_{t_1}, .., z_{t_T}$)
- Optionally, a sequence of -usually deterministic- T inputs $u_{1:T} = \{(u_t)_{t=1,...,T}\} \in \mathbb{R}^U$ (resp. $u_{t_i}, i = 1, ..., T$)
- **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 $q_\phi(z_{1:T}|x_{1:T})$ (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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Likelihood

- Observation model and encoder:

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

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

- Log likelihood

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

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

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

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

Likelihood

- Observation model and encoder:

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

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Variational Lower Bound

- Lower bound:

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

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

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

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

- 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_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

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

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

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

First model : Deep Kalman Filter

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

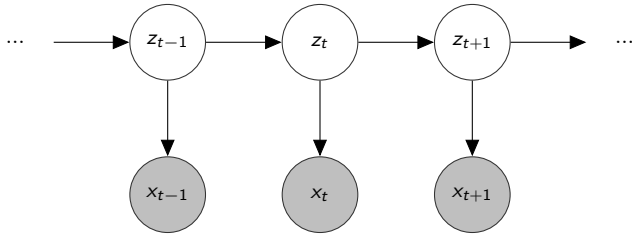


Figure: Probabilistic model of a Deep Kalman Filter

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:

$$p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}) = p_{\theta_x}(x_t|z_t) \tag{14}$$
$$p_{\theta_z}(z_t|z_{1:t-1}, x_{1:t}) = p_{\theta_z}(z_t|z_{t-1}) \tag{15}$$
$$q_\phi(z_t|z_{1:t-1}, x_{1:T}) = q_\phi(z_t|z_{t-1}, x_{t:T}) \tag{16}$$

Deep Kalman Filter - generative model - 2

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

$$p_{\theta_x}(x_t|z_t) = \mathcal{N}(x_t|\mu_{\theta_x}(z_t), \text{diag}\,\sigma^2_{\theta_x}(z_t)) \tag{17}$$
$$p_{\theta_z}(z_t|z_{t-1}) = \mathcal{N}(z_t|\mu_{\theta_z}(z_{t-1}), \text{diag}\,\sigma^2_{\theta_z}(z_{t-1})) \tag{18}$$
$$q_\phi(z_t|z_{t-1}, x_{t:T}) = \mathcal{N}(z_t|\mu_\phi(z_{t-1}, x_{t:T}), \text{diag}\,\sigma^2_{\theta_z}(z_{t-1}, x_{t:T})) \tag{19}$$

- 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:

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

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

Deep Kalman Filter - summary

Deep Kalman Filter

- **generative model**

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

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

- **inference model**

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

- **VLB for training**

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

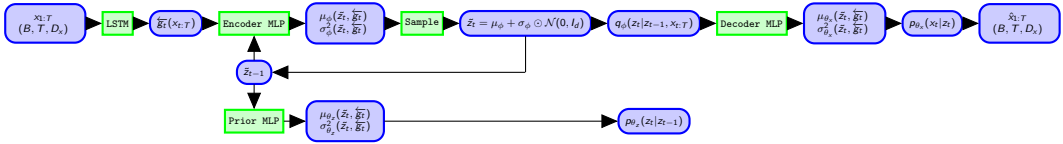
DKF - Torch

- The $\mathbb{KL}\left(q_\phi || p_{\theta_z}\right)$'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:

$$\overleftarrow{g_t} = \text{Backward LSTM}(\overleftarrow{g_{t+1}}, x_t) \text{ (encodes } x_{t:T})$$
$$q_\phi(z_t|z_{t-1}, x_{t:T}) = \mathcal{N}(z_t|\mu_\phi(z_{t-1}, \overleftarrow{g_t}), \text{diag}\, \sigma^2_\phi(z_{t-1}, \overleftarrow{g_t}))$$

DKF - Torch - Schematic blocks

The PyTorch implementation is described below:



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

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.

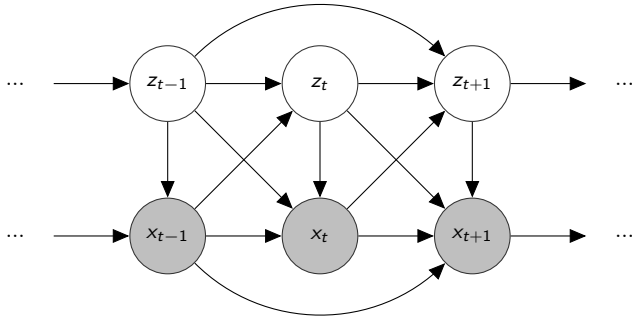


Figure: Probabilistic model of a Variational RNN

VRNN - Summary

Variational RNN

- **generative model**

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

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

- **inference model**

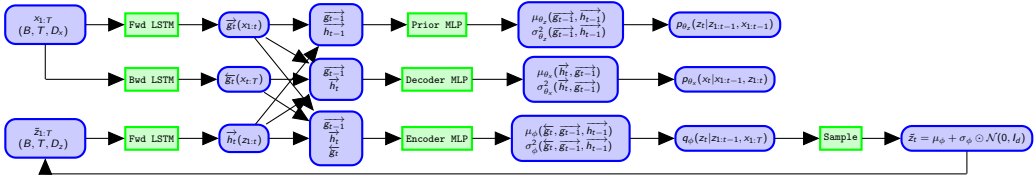
$$q_\phi(z_t|z_{1:t-1}, x_{1:T}) = \mathcal{N}(z_t|\mu_\phi(z_{1:t-1}, x_{1:T}), \text{diag}\, \sigma^2_\phi(z_{1:t-1}, x_{1:T})) \tag{28}$$

- **VLB for training**

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

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.



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

Third model : Gaussian Process - Variational Auto Encoder

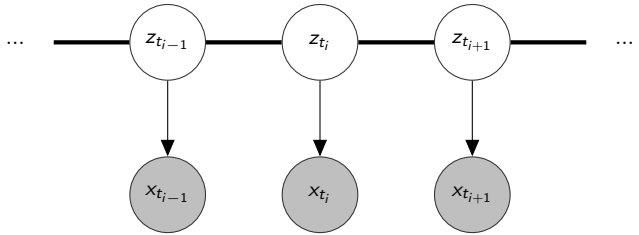


Figure: Probabilistic model of a GP-VAE

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

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

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 $l \in \{1, ..., L\}$ of the latent variables.** Formally:

$$p_{\theta_z}(z^l_{t_1:t_T}) = \mathcal{GP}(m_{\theta_z,l}(t_1 : t_T), k_{\theta_z,l}(t_1 : t_T, t_1 : t_T)) \qquad l = 1, .., L \tag{31}$$

  - $m_{\theta_z,l}$ 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 :

$$q_\phi(z^l_{t_1:t_T}|x^l_{t_1:t_T}) = \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Sigma^l_\phi(x_{t_1:t_T})) \qquad l = 1, .., L \tag{32}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Lambda^l_\phi(x_{t_1:t_T})^{-1}) \tag{33}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), L^l_\phi(x_{t_1:t_T}) L^l_\phi(x_{t_1:t_T})^T) \tag{34}$$

Code covariance with covariance matrix Σ^l_ϕ, precision matrix Λ^l_ϕ, or with a Cholesky decomposition $L^l_\phi L^l_\phi$.

GP-VAE generative model

From [15]

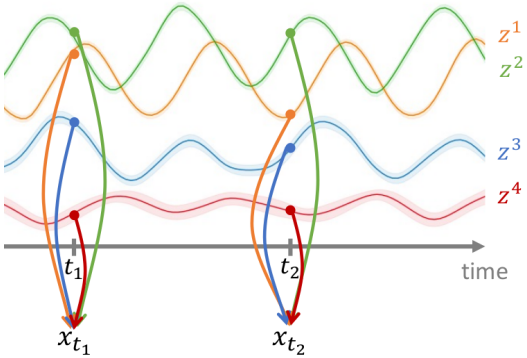


Figure: GP-VAE Schematics

GP-VAE likelihood and ELBO

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

We note that:

- the $\mathbb{KL}$-divergence is the sum of the L $\mathbb{KL}$-divergences $\mathbb{KL}\left(q^l_\phi||p^l_{\theta_z}\right)$ (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 $t_1, ...t_T$. ($O(N^3)$ 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

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

$$p_{\theta_z}(z^l_{t_1:t_T}) = \mathcal{GP}(m_{\theta_z,l}(t_1 : t_T), k_{\theta_z,l}(t_1 : t_T)) \qquad l = 1, .., L \tag{37}$$

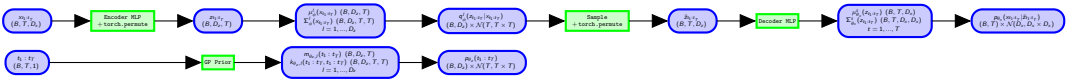
$$q_\phi(z^l_{t_1:t_T}|x^l_{t_1:t_T}) = \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Sigma^l_\phi(x_{t_1:t_T})) \qquad l = 1, .., L \tag{38}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Lambda^l_\phi(x_{t_1:t_T})^{-1}) \tag{39}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), L^l_\phi(x_{t_1:t_T}) L^l_\phi(x_{t_1:t_T})^T) \tag{40}$$

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

GP-VAE - Torch



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

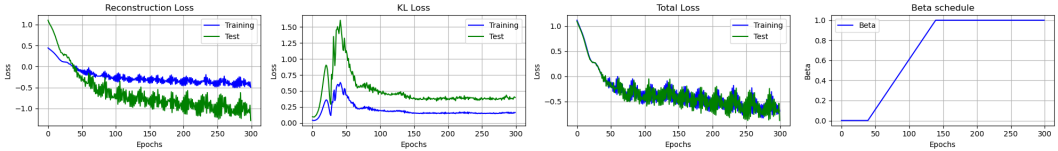
Code

GitHub repo

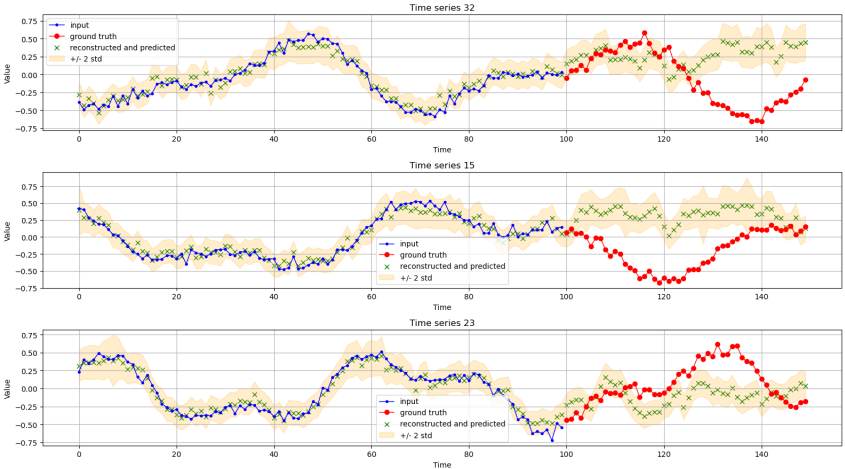
All code at Benjamin GitHub repo

DKF - Toy training - Loss

- **Posterior collapse !**
- Need β schedule (weight between reconstruction loss and $\mathbb{KL}$)

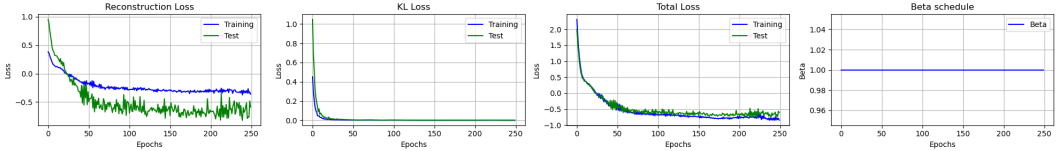


DKF - Toy training - Generations

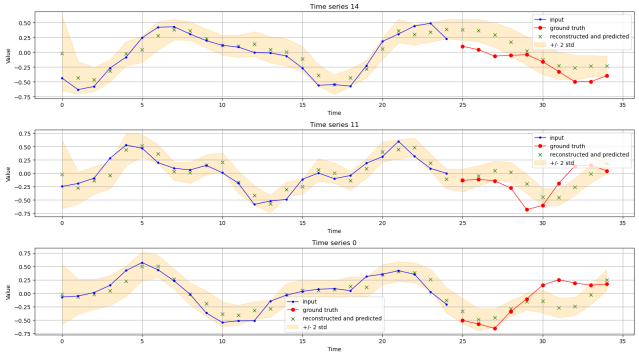


VRNN - Toy training - Loss

- 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 possibles values each
  - 3 possible poses (left, front, right)
- Motion accross time : 3 possible actions (walk, spell, slash) accross 8 consecutive frames.

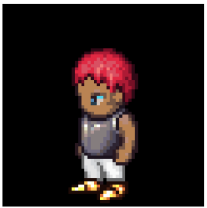
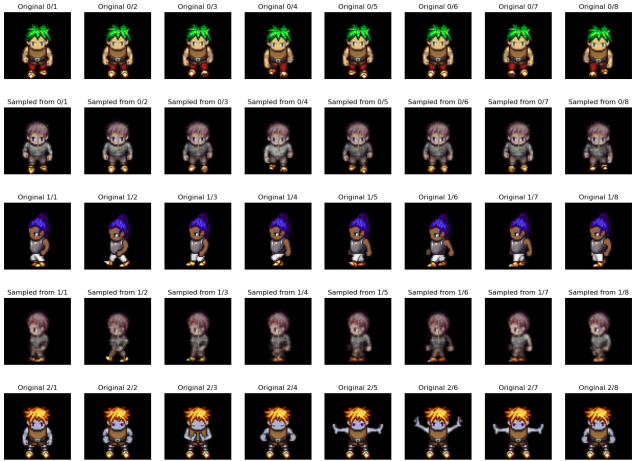


Figure: One sprite

Sprites series

VRNN Reconstruction on Sprites



VRNN Generation

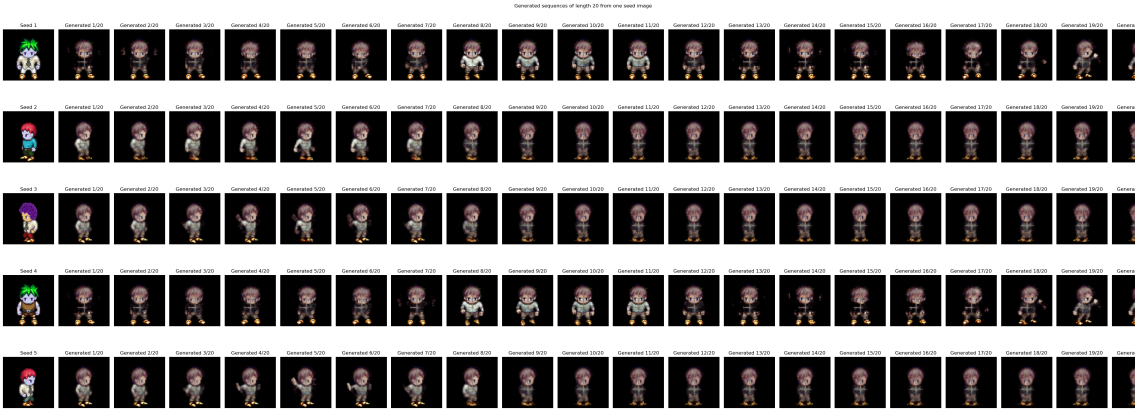
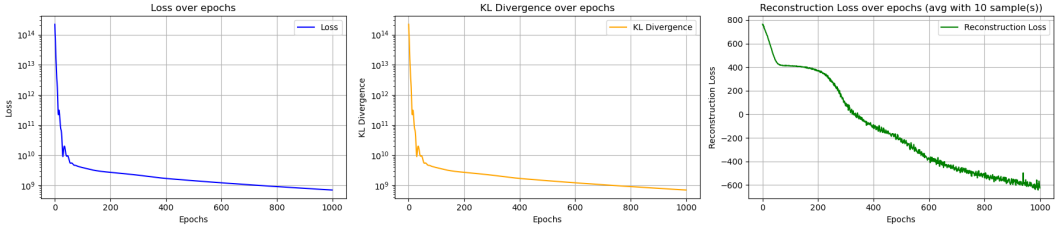


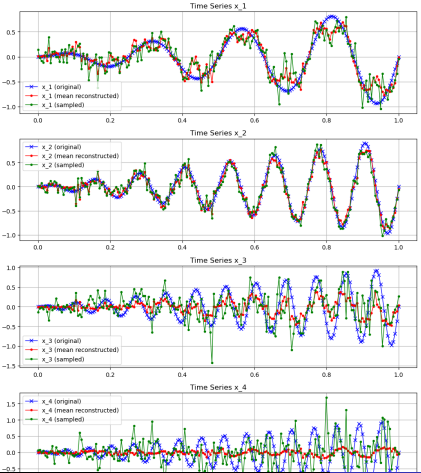
Figure: VRNN Sprites generation

GPVAE - Toy training - Loss

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

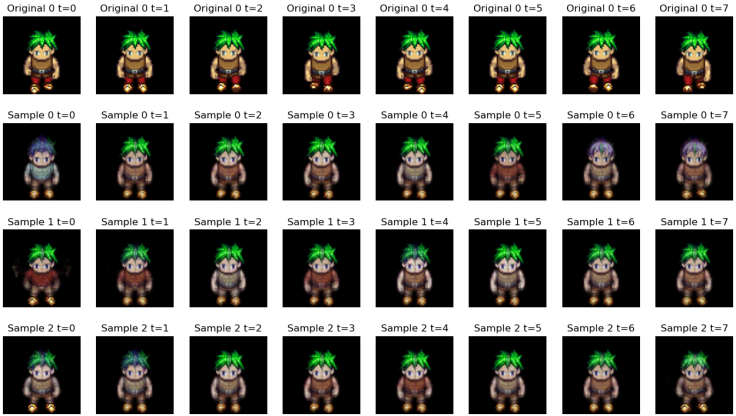


GPVAE - Toy training - Generations



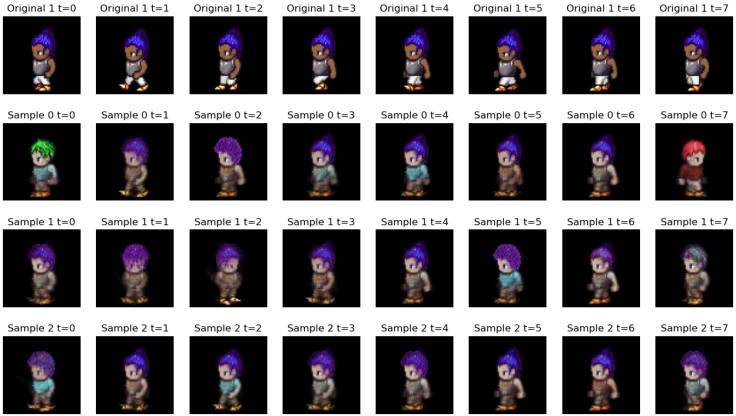
GPVAE - Sprites Reconstruction - 1

Top: original, below: reconstructions



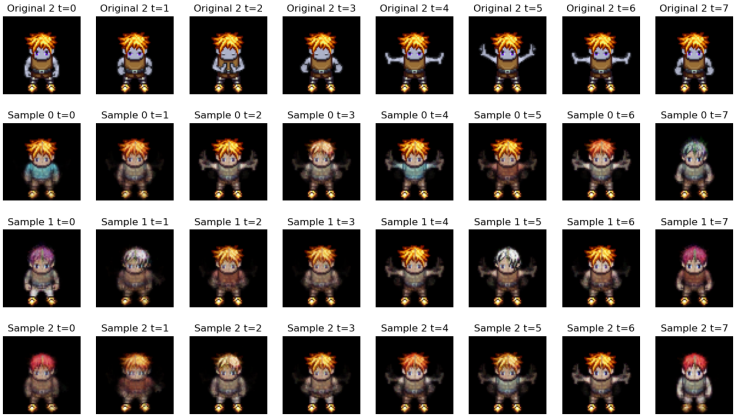
GPVAE - Sprites Reconstruction - 2

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) !!

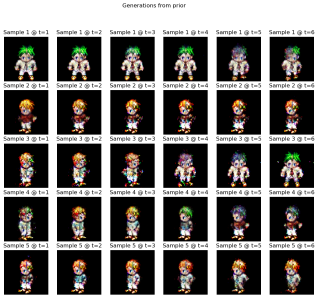


Figure: GPVAE Sprites generation 1

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

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

[a] 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 $[s, t]$ (equiped with a subdivison $\pi = \{s = t_0 < t_1 < ... < t_k < ... < t_n = t\}$), and defined as the limit when $|\pi| \to 0$ of $V_\pi^{(2)} = \sum_{k=0}^{n-1} |f(t_{k+1}) - f(t_k)|^2$, is:

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

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:

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

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 $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}, (x, t) \mapsto f(x, t)$ 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:

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

The last term is Itô's complementary term.
In dimension $d > 1$:

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

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** $F : \mathbb{R}^D \times \mathbb{R} \to \mathbb{R}^{D \times D}$
- L be a deterministic function **diffusion** (aka dispersion) $L : \mathbb{R}^D \times \mathbb{R} \to \mathbb{R}^{D \times S}$

The SDE is:

$$dX_t = F(X_t, t)dt + L(X_t, t)dB_t \tag{46}$$
$$X_{t_0} = X_0 \tag{47}$$

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:

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

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:

$$dX_t = F(t)X_t dt + L(t)dB_t \tag{48}$$
$$X_{t_0} = X_0 \sim \mathcal{N}(m_0, P_0) \tag{49}$$

Transition kernels for linear SDEs

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

$$\Psi : \mathbb{R}^2 \to \mathbb{R}^D \tag{50}$$

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

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

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

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

$$\Psi(t, t) = I_d \tag{55}$$

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

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

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

$$dZ_t = F(Z_t, t)dt + L(Z_t, t)dB_t \tag{58}$$
$$x_k \sim p(x_k|z_{t_k}) \tag{59}$$

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

$$dZ_t = F(t)Z_t dt + L(t)dB_t \tag{60}$$
$$dX_t = H(t)X_t dt + d\eta_t \tag{61}$$

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

$$p(z_t|x_{<t}) = \mathcal{N}(Z_t|m_t, P_t) \tag{62}$$
$$K = PH(t)^T R^{-1} \tag{63}$$
$$dm = F(t)mdt + K(dX_t - H(t)mdt) \tag{64}$$
$$\frac{dP}{dt} = F(t)P + PF(t)^T + L(t)QL(t)^T - KRK^T \tag{65}$$

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:

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

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

- 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:

$$dZ_t = F(t)Z_t dt + L(t)dB_t \tag{70}$$

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

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

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

- becomes in continuous time:

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

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

Latent ODE - model

- Generative model

$$z_{t_0} \sim p_{\theta_z}(z_{t_0}) \tag{74}$$
$$z_{t_1}, z_{t_2}, ..., z_{t_N} = \text{ODE Solver}(z_{t_0}, f, \theta_f, t_0, ..., t_N) \tag{75}$$
$$x_{t_i} \sim p_{\theta_x}(x_t|z_t) \tag{76}$$

- Inference

$$[\mu_\phi, \Sigma_\phi] = \text{LSTM}(x_{t_0:t_N}) \tag{77}$$
$$q_\phi(z_{t_0}|x_{t_0:t_N}) = \mathcal{N}(z_{t_0}|\mu_\phi, \Sigma_\phi) \tag{78}$$

Latent ODE - model

We reproduce here the drawing from the paper:

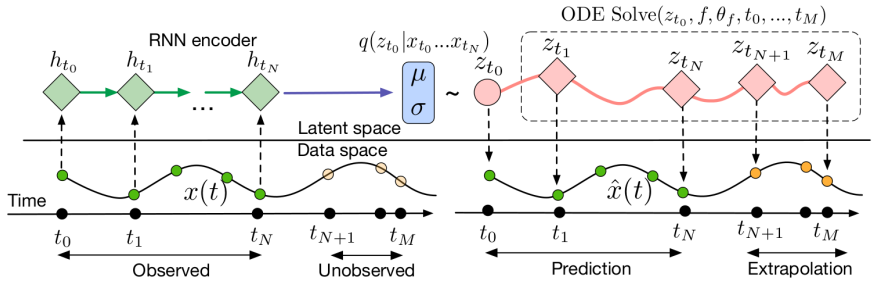


Figure: Neural ODE model

Latent ODE - ELBO

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

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

- likelihood:

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

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

- Need to compute the gradients of $\log p_{\theta_x}(x_{t_i}|z_{t_i})$ w.r.t. θ_f. Methods are forward sensivity, backpropragation 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 intial 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:

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

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

Which leads to an SDE prior:

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

$$Z_{t_0} \sim Z_0 \tag{85}$$

(where we used σ_θ 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 $z_t - z_{t_0} = \int_{t_0}^{t} f_\theta(Z_t, t)dt + \int_{t_0}^{t} \sigma_\theta(Z_t, t)d\tilde{B}_t$

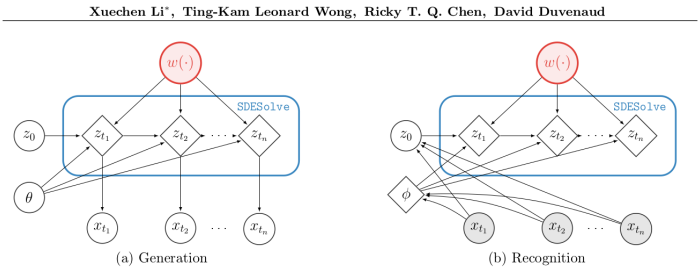
Latent SDE - generative model

The approximate posterior can also be described as a SDE:

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

$$Z_{t_0} = z_0 \text{ from prior} \tag{87}$$

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



(a) Generation (b) Recognition

Latent SDE - inference

- neural networks to learn the drift f_ϕ and the diffusion σ_θ
- requires to compute the gradient of functionals (loss) of type:

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

  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:

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

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