Dynamical Variational Autoencoders (discrete and continuous) Links to stochastic calculus and stochastic differential equations

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Summary

Abstract

- **Data sequences** : we consider data sequences $(X_t)_{t\in\mathbb{T}} \in \mathbb{R}^D$, where $\mathbb{T}$ is a set of times, either discrete or continuous. ie : time-series, videos, motion captures, patient data...
- **Dynamical Variational Auto Encoders** are a class of VAE models in which some structure is given to the latent variables to express the time dependency of the X_t.
- **Discrete-time DVAEs** are a large set of models, from the well-known Kalman filter up to the Variational RNN. We review the Deep Kalman filter and the VRNN models.
- **Continuous-time DVAEs** use a continuous prior over the latent variables, which allows to deal with irregularly sampled data, or data with missing components. We review the Gaussian Process VAE.
- **Stochastic calculus and stochastic differential equations** provides an elegant mathematical framework for DVAEs. We give a survival kit on stochastic calculus and SDEs.
- **The solution of a linear SDE is a Gaussian process** : we can use known filtering and smoothing Kalman algorithms to **compute the GP regression (ie posterior distribution) in GP-VAE with a linear cost.**
- **Beyond GP : Latent SDE model** - Not all Gaussian Processes are the solution to a linear SDE. Also, if the solution of a general SDE is a Markov process, it is not necessarily a Gaussian process. This leads to considering Latent SDE model, where the latent prior is a general SDE.

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Dynamical Variational Auto Encoders : what is it ?

- **Dynamical Variational Auto Encoders** are a class of VAEs in which some structure is given to the latent variables to encode the time dependency.
- DVAEs can be discrete-time or continuous models, can require regularly-sampled data, or can manage irregularly sampled data.
- For example, a Kalman filter is the simplest DVAE :
  - first order Markov chain for latent variables
  - linear Gaussian observation model.
- As in vanilla VAEs, inference is performed by evidence lower bound maximization.
- Notations

  - the data is a sequence of T points noted $x_{1:T} = \{(x_t)_{t=1,\dots,T}\} \in \mathbb{R}^F$.
  - the sequence of the associated T latent variables is $z_{1:T} = \{(z_t)_{t=1,\dots,T}\} \in \mathbb{R}^L$
  - optionally, there may be a sequence of -usually deterministic- T inputs $u_{1:T} = \{(u_t)_{t=1,\dots,T}\} \in \mathbb{R}^U$

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General formulation of DVAE

Generative model

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

The only assumption that is made is a a causal dependency of the x_t, z_t on the inputs $u_{1:t}$, thus allowing to change the conditioning $|u_{1:T}$ into $|u_{1:t}$.
In the rest of the presentation, we will consider systems with no input, and drop the conditioning on $u_{1:t}$ to simplify notations. However, the reasoning remains the same with inputs.

Posteriors

- The true posterior $p(z_{1:T}|x_{1:T})$ is usually untractable, but can be developed:

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

- As in vanilla Variational Auto Encoders (VAEs), the inference model is the approximation of the true posterior by an parametric encoder $q_\phi(z_{1:T}|x_{1:T})$, where ϕ is the set of parameters:

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- Depending on the chosen graphical models and the corresponding D-separation results, the observation model $p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}, u_{1:t})$ (with θ_x the set of parameters of the observation model) and approximate posterior $q_\phi(z_t|z_{1:t-1}, x_{1:T})$ will simplify.
- It is also considered a good practice to copy the expression of $q_\phi(z_t|z_{1:t-1}, x_{1:T})$ from the expression of the true posterior resulting from the D-separation analysis (see next chapters for examples).

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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

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

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

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

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

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Variational Lower Bound

- Lower bound:

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

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

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

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

- The first term is the usual **reconstruction error**.
- The second term is a regularization term, summing over the time steps the average divergence between the approximate posterior distribution of the latent variable at time t, and its real distribution.
- As in vanilla VAE, the sampling over q_ϕ requires the use of the "re parametrization trick" (see [?]), 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

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

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

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

Deep Kalman Filter

Deep Kalman Filter Directed Acyclic Graph (DAG):

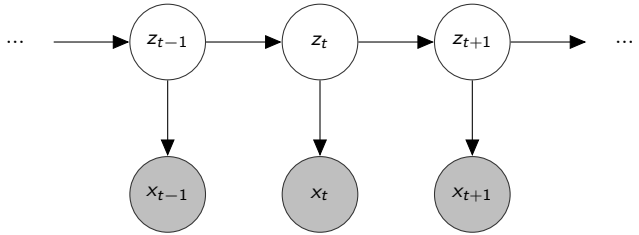


Figure: Probabilistic model of a Deep Kalman Filter

Deep Kalman Filter - generative model

Using **D-separation** on the DAG to simplify the general Dynamical Variational Auto Encoder (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

We then choose Gaussian distributions for $p_{\theta_x}, p_{\theta_z}$ and q_ϕ, with 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, as it has the same formulation as the true posterior and respects the corresponding dependencies.

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**

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

- **Variational Lower Bound (VLB) for training**

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

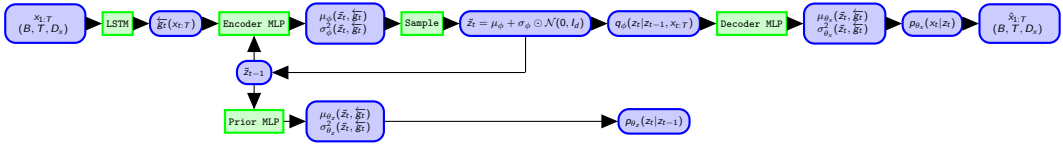
DKF - Torch

- The $\mathbb{KL}\left(q_\phi || p_{\theta_z}\right)$'s have a close form, as the two distributions are Gaussians (see **??**)
- Following [**?**], we use forward Long Short Term Memory (LSTM) to encode sequences such as $x_{1:t}$, and backward LSTM to encode sequences such as $x_{t:T}$, as inputs into 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

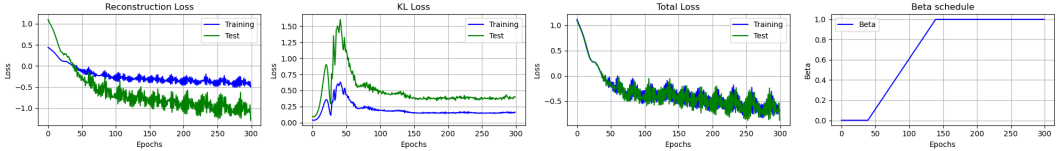
The PyTorch implementation is described below:



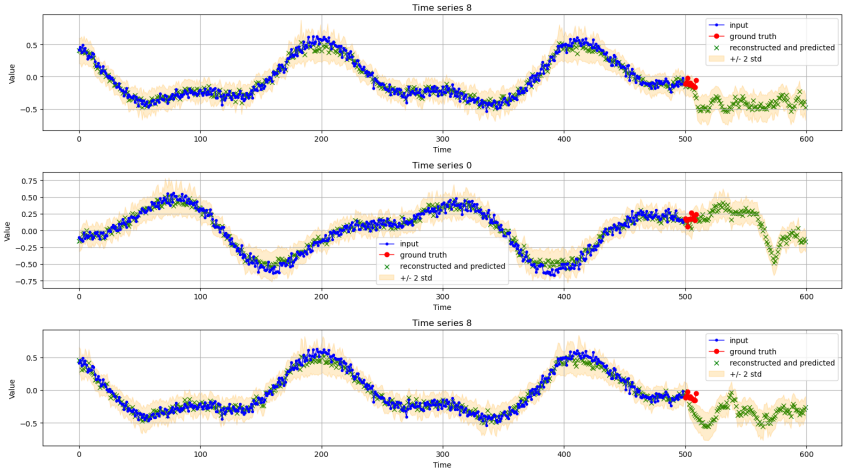
$$\mathcal{L}(\theta, \phi, X) = \sum_{t=1}^{T} \mathbb{E}_{q_\phi(z_t|x_{1:T})} \log p_{\theta_x}(x_t|z_t) - \sum_{t=1}^{T} \mathbb{E}_{q_\phi(z_{t-1}|x_{1:T})} \mathbb{KL}\left(q_\phi(z_t|z_{t-1}, x_{t:T}) || p_{\theta_z}(z_t|z_{t-1})\right)$$

DKF - Toy training - Loss

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



DKF - Toy training - Generations



Variational RNN

The Variational Recurrent Neural Network (VRNN) is the most expressive DVAE, in that sense that the general expressions 11, 12 and VLB 13 can not be simplified.
The Graphical Probabilistic Model (GPM) of the VRNN assumes full connections between latent variables, and between observed variables, to account for the full unsimplified expressions. Specifically:

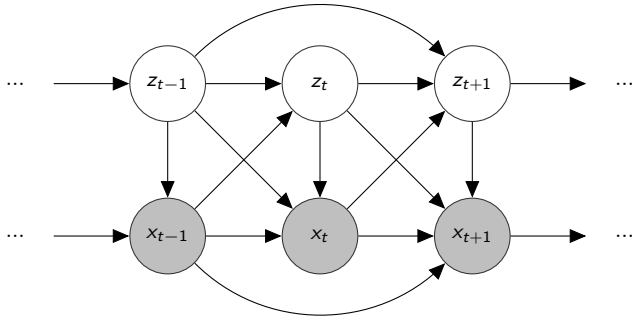


Figure: Probabilistic model of a Variational RNN

VRNN - Summary

Variational RNN

- **generative model**

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

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

- **inference model**

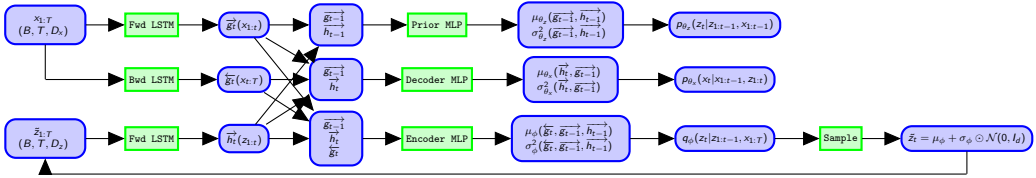
$$q_\phi(z_t|z_{1:t-1}, x_{1:T}) = \mathcal{N}(z_t|\mu_\phi(z_{1:t-1}, x_{1:T}), \text{diag}\, \sigma^2_\phi(z_{1:t-1}, x_{1:T})) \tag{28}$$

- **VLB for training**

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

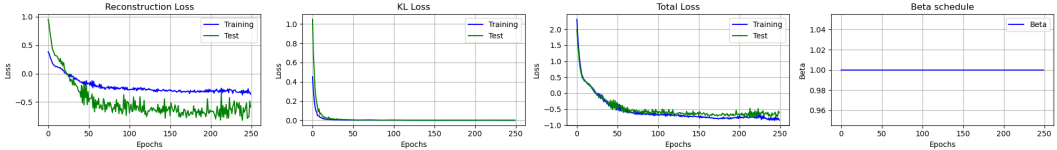
VRNN - Torch

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

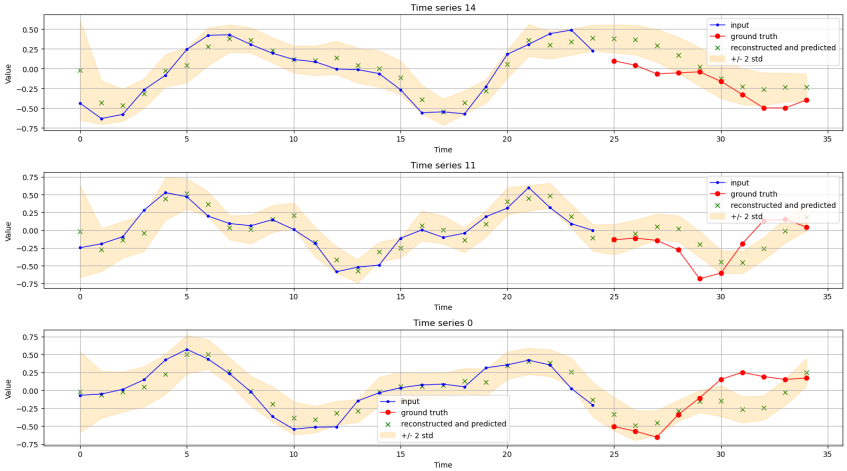


$$\mathcal{L}(\theta, \phi, X) = \sum_{t=1}^{T} \mathbb{E}_{q_\phi(z_{1:t}|x_{1:T})} \log p_{\theta_x}(x_t|x_{1:t-1}, z_{1:t}) - \sum_{t=1}^{T} \mathbb{E}_{q_\phi(z_{1:t-1}|x_{1:T})} \mathbb{KL}\left(q_\phi(z_t|z_{1:t-1}, x_{1:T}) || p_{\theta_z}(z_t|z_{1:t-1}, x_{1:t-1})\right)$$

VRNN - Toy training - Loss



VRNN - Toy training - Generation



Gaussian Process - Variational Auto Encoder

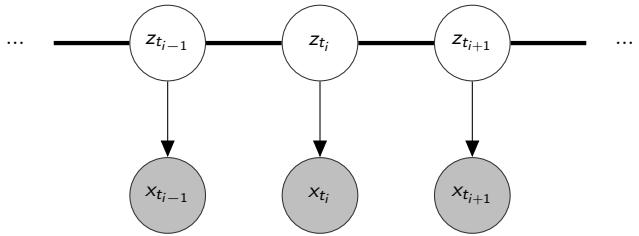


Figure: Probabilistic model of a GP-VAE

- The thick black lines indicate all latent variables follow a Gaussian Process.
- The joint distribution writes somehow differently from the one for DVAEs, as:

$$p(x_{t_1:t_T}, z_{t_1:t_T}) = p(z_{t_1:t_T})p(x_{t_1:t_T}|z_{t_1:t_T}) \tag{30}$$

$$= p(z_{t_1:t_T}) \prod_{i=1}^{T} p(x_{t_i}|x_{t_1:t_{i-1}}, z_{t_1:t_T}) \tag{31}$$

$$= \prod_{i=1}^{T}$$

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:

$$p_{\theta_z}(z^l_{t_1:t_T}) = \mathcal{GP}(m_{\theta_z,l}(t_1 : t_T), k_{\theta_z,l}(t_1 : t_T, t_1 : t_T)) \qquad l = 1, .., L \tag{33}$$

  where the $m_{\theta_z,l}$ are the L mean functions of the Gaussian Process (GP) priors (usually chosen constant null), and the $k_{\theta_z,l}$ are the kernel functions of the GP priors.
  - by design, each of the component of the z_{t_i} is a scalar GP, with correlation over time stamps. However, the different components of a z_{t_i} are not correlated between them. The correlation across dimensions is encoded into the observation model $p_{\theta_x}(x_{t_i}|z_{t_i})$.
  - the kernels $k_{\theta_z,l}$ can be chosen differently to account for different prior knowledge of the data sequence. In [?] for example, Fortuin and al. uses a set of Gaussian Kernels with different lenghtscales.
- **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 :

$$q_\phi(z^l_{t_1:t_T}|x^l_{t_1:t_T}) = \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Sigma^l_\phi(x_{t_1:t_T})) \qquad l = 1, .., L \tag{34}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Lambda^l_\phi(x_{t_1:t_T})^{-1}) \tag{35}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), L^l_\phi(x_{t_1:t_T}) L^l_\phi(x_{t_1:t_T})^T) \tag{36}$$

  where we have made explicit the different ways of defining the multivariate normal distribution, with its covariance matrix Σ^l_ϕ, its precision matrix Λ^l_ϕ, or with a Cholesky decomposition $L^l_\phi L^l_\phi$.

GP-VAE likelihood and ELBO

$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^{T} \mathbb{E}_{q_\phi(z_{t_i}|x_{t_1:t_T})} \log p_{\theta_x}(x_{t_i}|z_{t_i}) - \mathbb{KL}\left(q_\phi(z_{t_1:t_T}|x_{t_1:t_T})||p_{\theta_z}(z_{t_1:t_T})\right) \tag{37}$$

We note that:

- the $\mathbb{KL}$-divergence is actually the sum of the L $\mathbb{KL}$-divergences $\mathbb{KL}\left(q^l_\phi||p^l_{\theta_z}\right)$, which have a close form solution as both distributions are Gaussian. (see the well-known result **??**)
- the reconstruction 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 $t_1, ...t_T$. If the kernel parameters are fixed -such as in [**?**]- 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 [**?**]), then the computation must occur at each training iteration.

GP-VAE Summary

Gaussian Process VAEs

$$p(x_{t_1:t_T}, z_{t_1:t_T}) = p(z_{t_1:t_T}) \prod_{i=1}^{T} p(x_{t_i}|z_{t_i}) \tag{38}$$

$$p_{\theta_z}(z^l_{t_1:t_T}) = \mathcal{GP}(m_{\theta_z,l}(t_1 : t_T), k_{\theta_z,l}(t_1 : t_T)) \qquad l = 1, .., L \tag{39}$$

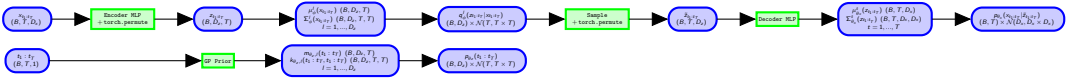
$$q_\phi(z^l_{t_1:t_T}|x^l_{t_1:t_T}) = \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Sigma^l_\phi(x_{t_1:t_T})) \qquad l = 1, .., L \tag{40}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), \Lambda^l_\phi(x_{t_1:t_T})^{-1}) \tag{41}$$

$$= \mathcal{N}(m^l_\phi(x_{t_1:t_T}), L^l_\phi(x_{t_1:t_T}) L^l_\phi(x_{t_1:t_T})^T) \tag{42}$$

$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^{T} \mathbb{E}_{q_\phi(z_{t_i}|x_{t_1:t_T})} \log p_{\theta_x}(x_{t_i}|z_{t_i}) - \mathbb{KL}\left(q_\phi(z_{t_1:t_T}|x_{t_1:t_T})||p_{\theta_z}(z_{t_1:t_T})\right) \tag{43}$$

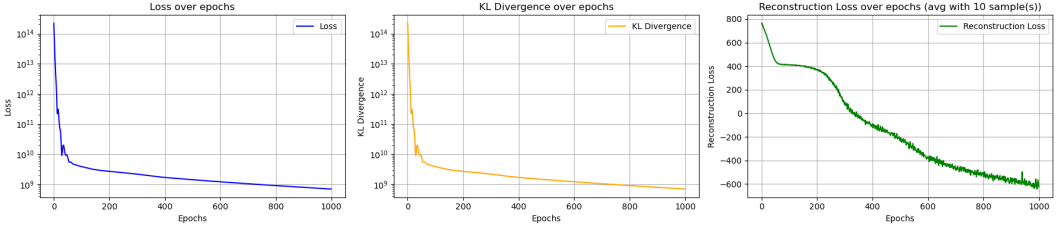
GP-VAE - Torch



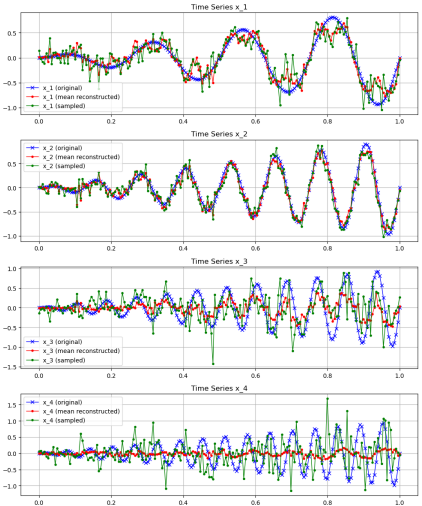
$$\mathcal{L}(\theta, \phi, X) = \sum_{i=1}^{T} \mathbb{E}_{q_\phi(z_{t_i}|x_{t_1:t_T})} \log p_{\theta_x}(x_{t_i}|z_{t_i}) - \mathbb{KL}\left(q_\phi(z_{t_1:t_T}|x_{t_1:t_T})||p_{\theta_z}(z_{t_1:t_T})\right)$$

GPVAE - Toy training - Loss

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



GPVAE - Toy training - Generations



Stochastic calculus survival kit - Stochastic process

Definition

A **stochastic process** is defined as:

$$X = (\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\in T}, (X_t)_{t\in T}, \mathbb{P}) \tag{44}$$

where:

- Ω is a set (universe of possibles).
- $\mathcal{F}$ is a σ-algebra of parts of Ω
- $\mathbb{P}$ is a probability measure on $(\Omega, \mathcal{F})$
- $T \subset \mathbb{R}_+$ represents time
- $(\mathcal{F}_t)_{t\in T}$ is a **filtration**, ie an increasing family of sub-σ-algebras of $\mathcal{F}$ indexed by t : $\forall 0 \leq s \leq t \in T$, $\mathcal{F}_s \subset \mathcal{F}_t \subset \mathcal{F}$.
- $(X_t)_{t\in T}$ is a family of RV defined on $(\Omega, \mathcal{F})$ with values in a measurable space $(E, \mathcal{E})$ or more simply $(E, \mathcal{B}(E))$ (set E endowed with its Borelian σ-algebra).
- $(X_t)_{t\in T}$ is assumed **adapted to the filtration** $(\mathcal{F}_t)_{t\in T}$, meaning $\forall t \in T$, X_t is $\mathcal{F}_t$-measurable

A filtration $\mathcal{F}_{t\geq 0}$ is often viewed and introduced as the *set of information available at time t*.

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 [?]

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:

$$\lim_{|\pi|\to 0} V_\pi^{(2)} = Q(t-s) \text{ in } L^2 \tag{45}$$

Stochastic calculus survival kit - Stochastic Integrals

Ito then proceeds to define **stochastic integrals**, starting with elementary processes:

Definition

A stochastic process $X = (X_s)_{s\in[a,b]}$ is called **elementary** if there exists a subdivision $a = t_0 < t_1 < ... < t_n = b$ of $[a, b]$, such that:

$$\forall t \in [a, b], \forall \omega \in \Omega, X_t(\omega) = \sum_{i=0}^{n-1} X_i(\omega)\mathbf{1}_{[t_i,t_{i+1}[}(t)$$

with $\forall i \in \{0, 1, .., n-1\}, X_i$ is $\mathcal{F}_{t_i}$-measurable.
This means that, in each interval $[t_i, t_{i+1}[$, $X_t(\omega)$ is independent of t and $X_t(\omega) = X_i(\omega)$.
We define $\mathcal{E}$ (resp. $\mathcal{E}_n, n > 0$) the set of all elementary processes on $[a, b]$ (resp. the subset of the $X \in \mathcal{E}$) such that all X_i have a finite moment $\mathbb{E}X_i < \infty$ (resp $\mathbb{E}(|X_i|^n) < \infty$).

Stochastic calculus survival kit - Stochastic Integrals 2

Definition

Let $X \in \mathcal{E}$, ie

$$X_t(\omega) = \sum_{i=0}^{n-1} X_i(\omega) \mathbf{1}_{[t_i, t_{i+1}[}(t)$$

The stochastic integral of X is the real random variable :

$$\int_a^b X_t dB_t := \sum_{i=0}^{n-1} X_i (B_{t_{i+1}} - B_{t_i})$$

The notion is then extended to other stochastic processes (in spaces of square integrable processes, see the annex).

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:

$$X_t = X_0 + \int_0^t a_s ds + \int_0^t b_s dB_s \ \ \forall t \in [0,T] \tag{46}$$

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 soltuion 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:

$$d\left(f(X_t, t)\right) = \frac{\partial f}{\partial t}(X_t, t)dt + \frac{\partial f}{\partial x}(X_t, t)dX_t + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(X_t, t)b_t^2 dt \tag{47}$$

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

$$d\left(f(X_t, t)\right) = \frac{\partial f}{\partial t}(X_t, t)dt + (\nabla f)^T(X_t, t)dX_t + \frac{1}{2}Tr\left((\nabla\nabla^T f)dX_t dX_t^T\right) \tag{48}$$

Defintion 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 "dispersion" $L : \mathbb{R}^D \times \mathbb{R} \to \mathbb{R}^{D \times S}$

The Stochastic Differential Equation (SDE) is:

$$dX_t = F(X_t, t)dt + L(X_t, t)dB_t \tag{49}$$
$$X_{t_0} = X_0 \tag{50}$$

where X_0 can be a scalar constant or a random variable. A stochastic process X is said to be solution of 49 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 49 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 [**?**].)

Transition Kernels

- Formally, a Markov process is caracterized by its **transition kernels**.
- That is, for any $s < t$, and any $A \in \mathcal{B}_{\mathbb{R}^D}$, a Markov process verifies $\mathbb{P}(X_t \in A|\mathcal{F}_s) = \mathbb{P}(X_t \in A|X_s)$.
- the transition kernels of X are the applications $P_{s,t} : \mathbb{R}^D \times \mathcal{B}_{\mathbb{R}^D} \to [0,1]$, such that for any $f : \mathbb{R}^D \to \mathbb{R}$ measurable and bounded, we have:

$$P_{s,t}f(x) = \int_{\mathbb{R}^D} P_{s,t}(x, dy)f(y) \tag{51}$$

So $P_{s,t}$ actually is the probability measure of starting from x at time s, and reach $y \in dy$ at time t.

When the transition kernels have densities $p(x, t|y, s)$ (ie starting from y at time s, and reaching x at time t), then a fundamental result is the **Fokker Plank Kolmogorov** equation (also known as forward Kolomogorov) :

$$\frac{\partial p}{\partial y} = \mathcal{A}^* p \tag{52}$$

$$\mathcal{A}^*(\bullet) = -\sum_{i=1}^{D} \frac{\partial}{\partial x_i}(F_i(x,t)(\bullet)) + \frac{1}{2}\sum_{i,j=1}^{D} \frac{\partial^2}{\partial x_i \partial x_j}(L(x,t)QL(x,t)^T|_{i,j}(\bullet)) \tag{53}$$

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 49:
The linear SDE is:

$$dX_t = F(t)X_t dt + L(t)dB_t \tag{54}$$
$$X_{t_0} = X_0 \sim \mathcal{N}(m_0, P_0) \tag{55}$$

Transition kernels for linear SDEs

In this case, the transition kernels family can be characterized as:

$$\Psi : \mathbb{R}^2 \to \mathbb{R}^D \tag{56}$$

$$\frac{\partial \Psi(\tau, t)}{\partial \tau} = F(\tau)\Psi(\tau, t) \tag{57}$$

$$\frac{\partial \Psi(\tau, t)}{\partial t} = -\Psi(\tau, t)F(t) \tag{58}$$

$$\Psi(\tau, t) = \Psi(\tau, s)\Psi(s, t) \text{ (Chapman-Kolmogorov)} \tag{59}$$

$$\Psi(\tau, t) = \Psi(t, \tau)^{-1} \tag{60}$$

$$\Psi(t, t) = I_d \tag{61}$$

The solution to a linear SDE 54 is a Gaussian Process:

$$X_t = \Psi(t, t_0)X_0 + \int_{t_0}^{t} \Psi(t, \tau)L(\tau)dB_\tau \tag{62}$$

$$X_{t_0} = X_0 \sim \mathcal{N}(m_0, P_0) \tag{63}$$

Beyond linear 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

$$dZ_t = F(Z_t, t)dt + L(Z_t, t)dB_t \tag{64}$$
$$x_k \sim p(x_k|z_{t_k}) \tag{65}$$

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

$$dZ_t = F(t)Z_t dt + L(t)dB_t \tag{66}$$
$$dX_t = H(t)X_t dt + d\eta_t \tag{67}$$

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

$$p(z_t|x_{<t}) = \mathcal{N}(Z_t|m_t, P_t) \tag{68}$$
$$K = PH(t)^T R^{-1} \tag{69}$$
$$dm = F(t)mdt + K(dX_t - H(t)mdt) \tag{70}$$
$$\frac{dP}{dt} = F(t)P + PF(t)^T + L(t)QL(t)^T - KRK^T \tag{71}$$

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

$$Z_{t_{k+1}} \sim p(Z_{t_{k+1}}|Z_{t_k}) \tag{72}$$
$$X_k \sim p(X_k|Z_{t_k}) \tag{73}$$

Bayesian smoother

$$Z_{t_{k+1}} \sim p(Z_{t_{k+1}}|Z_{t_k}) \tag{74}$$

$$X_k \sim p(X_k|Z_{t_k}) \tag{75}$$

The *Bayesian smoother* is, for any $k < T$:

$$p(Z_{t_{k+1}}|X_{1:k}) = \int p(Z_{t_{k+1}}|Z_{t_k}) p(Z_{t_k}|X_{1:k}) dZ_{t_k} \tag{76}$$

$$p(Z_{t_k}|X_{1:T}) = p(Z_{t_k}|X_{1:k}) \int \left(\frac{p(Z_{t_{k+1}}|Z_{t_k}) p(Z_{t_{k+1}}|X_{1:T})}{p(Z_{t_{k+1}}|X_{1:k}} dZ_{t_{k+1}} \right) \tag{77}$$

The backward recursion is started from the final step, where the filtering and smoothing densities are the same : $p(Z_{t_T}|X_{1:T})$.

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

- We wrap up here linking the filtering/smoothing theory of linear SDE with the Gaussian Process Variational Auto Encoder (GP-VAE) model of [**?**].
- Using the formalization above, a GP-VAE with Gaussian observation is basically:

$$Z_t \sim \mathcal{GP}(m(\bullet), k(\bullet, \bullet)) \tag{78}$$

$$X_{t_k} \sim \mathcal{N}(X_{t_k} | Z_{t_k}, \sigma^2) \tag{79}$$

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

$$dZ_t = F(t)Z_t dt + L(t)dB_t \tag{80}$$

$$X_{t_k} \sim \mathcal{N}(X_{t_k} | Z_{t_k}, \sigma^2) \tag{81}$$

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

Gaussian Processes as solutions of linear SDE

- **Brownian motion** : solution to $dZ_t = dB_t$, GP with kernel $k(t, t') = \min(t, t')$ (see **??**)
- **Ornstein Uhlenbeck** : the O.U. process

$$dZ_t = -\frac{1}{l} Z_t dt + dB_t \tag{82}$$

where dB_t has diffusion coefficient $\frac{2\sigma^2}{l}$, is a GP with kernel:

$$k_{\text{exp}} = \sigma^2 \exp\left(-\frac{|t - t'|}{l}\right) \tag{83}$$

- **Matern** : the SDE representation with

$$F = \begin{pmatrix} 0 & 1 \\ -\lambda^2 & -2\lambda \end{pmatrix}, L = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, H = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{84}$$

is a GP with the Matern kernel with $\nu = \frac{3}{2}$:

$$k_{\text{Matern}} = \sigma^2 \left(1 + \frac{\sqrt{3}|t - t'|}{l}\right) \exp\left(-\frac{\sqrt{3}|t - t'|}{l}\right) \tag{85}$$

and $\lambda = \frac{\sqrt{3}}{l}$, diffusion is $q = 4\lambda^3\sigma^2$.

Some Gaussian Processes are NOT solutions to linear SDE

Conversely, the following kernels can not be used to derive an associated linear SDE:

- **squared exponential** : the widely used

$$k_{\text{se}}(t, t') = \sigma^2 \exp\left(-\frac{|t - t'|^2}{2l^2}\right) \tag{86}$$

- **rational quadratic**:

$$k_{\text{rq}}(t, t') = \sigma^2 \left(1 + \frac{|t - t'|^2}{2\alpha l^2}\right)^{-\alpha} \tag{87}$$

with $\alpha > 0$.

In that latter case, one can use spectral decomposition (ie Mercer's theorem, see MVA kernel class [**?**]) to approximate the kernel function and determine an associated linear 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 continous-time priors.
- More general stochastic process priors can be used, expressed as solutions to general SDE : those are latent SDE models.

Next steps - next 3 weeks !

- Research/learning on models with other stochastic priors (neural SDEs ?)
- XPs : finding the right kernels for GP-VAE ?
- XPs : comparison between VRNN and GP-VAE on a common real life dataset ?
- Other ?