Neural Stochastic Differential Equations: 
Deep Latent Gaussian Models in the Diffusion Limit

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Abstract

In deep latent Gaussian models, the latent variable is generated by a time-inhomogeneous Markov chain, where at each time step we pass the current state through a parametric nonlinear map, such as a feedforward neural net, and add a small independent Gaussian perturbation. This work considers the diffusion limit of such models, where the number of layers tends to infinity, while the step size and the noise variance tend to zero. The limiting latent object is an Itô diffusion process that solves a stochastic differential equation (SDE) whose drift and diffusion coefficient are implemented by neural nets. We develop a variational inference framework for these neural SDEs via stochastic backpropagation in Wiener space, where the variational approximations to the posterior are obtained by Girsanov (mean-shift) transformation of the standard Wiener process and the computation of gradients is based on the theory of stochastic flows. This permits the use of black-box SDE solvers and automatic differentiation for end-to-end inference. Experimental results with synthetic data are provided.

1 Introduction

Ordinary differential equations (ODEs) and other types of continuous-time flows have always served as convenient abstractions for various deterministic iterative models and algorithms. Recently, however, several authors have started exploring the intriguing possibility of using ODEs for constructing and training very deep neural nets by considering the limiting case of composing a large number of infinitesimal nonlinear transformations [Haber and Ruthotto, 2017, Chen et al., 2018b, Li et al., 2018]. In particular, Chen et al. [2018b] have introduced the framework of neural ODEs, in which the overall nonlinear transformation is represented by an ODE, and a black-box ODE solver is used as a computational primitive during end-to-end training.

These ideas naturally carry over to the domain of probabilistic modeling. Indeed, since deep probabilistic generative models can be viewed as time-inhomogeneous Markov chains, we can consider the limit of infinitely many layers as a continuous-time Markov process. Since the marginal distributions of such a process evolve through a deterministic continuous-time flow, one can use ODE techniques in this context as well [Tabak and Vanden-Eijnden, 2010, Chen et al., 2018a]. However, an alternative possibility is to focus on the stochastic evolution of the sample paths of the limiting process, rather than on the deterministic evolution in the space of measures. This perspective is particularly useful when the generation of sample paths of the underlying process is more tractable than the computation of process distributions.

In this paper, we develop these ideas in the context of Deep Latent Gaussian Models (DLGMs), a flexible family of generative models introduced by Rezende et al. [2014]. In these models, the latent variable is generated by a time-inhomogeneous Markov chain, where at each time step we pass the current state through a deterministic nonlinear map, such as a feedforward neural net, and add a small
independent Gaussian perturbation. The observed variable is then drawn conditionally on the state of the chain after a large but finite number of steps. The iterative structure of DLGMs, together with the use of differentiable layer-to-layer transformations, is the basis of stochastic backpropagation [Kingma and Welling, 2014; Ranganath et al., 2014; Rezende et al., 2014], an efficient and scalable procedure for performing variational inference with approximate posteriors of the mean-field type. A key feature here is that all the randomness in the latent space is generated by sampling a large but finite number of independent standard Gaussian random vectors, and all other transformations are obtained by suitable differentiable reparametrizations.

If one considers the limiting regime of DLGMs where the number of layers tends to infinity, while the step size and the noise variance in layer-to-layer transformations both tend to zero, the resulting latent random object is a diffusion process of the Itô type [Bichteler, 2002; Protter, 2005], whose drift and diffusion coefficients are implemented by neural nets. We will refer to these models as neural SDEs, in analogy to the deterministic neural ODEs of Chen et al. [2018b]. Generative models of this type have been used considered in earlier work, first by Movellan et al. [2002] as a noisy continuous-time counterpart of recurrent neural nets, and, more recently, by Archambeau et al. [2007], Hashimoto et al. [2016], and Ryder et al. [2018]. On the theoretical side, Tzen and Raginsky [2019] have investigated the expressive power of diffusion-based generative models and showed that they can be used to obtain approximate samples from any distribution whose Radon–Nikodym derivative w.r.t. the standard Gaussian measure can be efficiently represented by a neural net. In this paper, we leverage this expressive power and develop a framework for variational inference in neural SDEs. Specifically, we make the following contributions:

- We show that all the latent randomness can be generated by sampling from the standard multidimensional Wiener process, in analogy to the use of independent standard Gaussian random vectors in DLGMs. Thus, the natural latent space for neural SDEs is the Wiener space of continuous vector-valued functions on [0, 1] equipped with the Wiener measure (the process law of the standard Wiener process).
- We derive a variational bound on the marginal log-likelihood for the observed variable using the Gibbs variational principle on the path space [Boué and Dupuis, 1998]. Moreover, any variational approximation to the posterior is related to the primitive Wiener process by a mean shift, by Girsanov’s theorem. Thus, the natural neural SDE counterpart of a mean-field approximate posterior is obtained by adding an observation-dependent neural net drift to the standard Wiener process.
- Finally, we show how variational inference can be carried out via stochastic backpropagation in Wiener space. To that end, we use the theory of stochastic flows [Kunita, 1984] in order to differentiate the solutions of Itô SDEs with respect to parameters of the drift and the diffusion coefficient. These pathwise derivatives are also solutions of Itô SDEs, whose drift and diffusion coefficients can be obtained from those of the original SDE using the ordinary chain rule of multivariable calculus. Thus, the overall process can be implemented using a black-box SDE solver and automatic differentiation.

While our focus is primarily theoretical, we provide proof-of-concept experimental results with synthetic data.

2 Background: variational inference in Deep Latent Gaussian Models

In Deep Latent Gaussian Models (DLGMs) [Rezende et al., 2014], the latent variables $X_0, \ldots, X_k$ and the observed variable $Y$ are generated recursively according to

$$X_0 = Z_0 \quad (1a)$$
$$X_i = X_{i-1} + b_i(X_{i-1}) + \sigma_i Z_i, \quad i = 1, \ldots, k \quad (1b)$$
$$Y \sim p(\cdot|X_k), \quad (1c)$$

where $Z_0, \ldots, Z_k \sim \mathcal{N}(0, I_d)$ are i.i.d. standard Gaussian vectors in $\mathbb{R}^d$, $b_1, \ldots, b_k : \mathbb{R}^d \to \mathbb{R}^d$ are some parametric nonlinear transformations, $\sigma_1, \ldots, \sigma_k \in \mathbb{R}^{k \times k}$ is a sequence of matrices, and $p(\cdot|\cdot)$ is the observation likelihood. Letting $\theta$ denote the parameters of $b_1, \ldots, b_k$ and the matrices $\sigma_1, \ldots, \sigma_k$, we can capture the underlying generative process by the joint probability density of $Y$. 

While our focus is primarily theoretical, we provide proof-of-concept experimental results with synthetic data.
and the ‘primitive’ random variables $Z_0, \ldots, Z_k$:  
\[ p_\theta(y, z_0, \ldots, z_k) = p(y | f_\theta(z_0, \ldots, z_k)) \phi_d(z_0) \cdots \phi_d(z_k), \quad (2) \]
where $f_\theta : \mathbb{R}^d \times \cdots \times \mathbb{R}^d \to \mathbb{R}^d$ is the overall deterministic transformation $(Z_0, \ldots, Z_k) \to X_k$ specified by (1a)-(1b), and $\phi_d(z) = (2\pi)^{-d/2} \exp(-\frac{1}{2} \|z\|^2)$ is the standard Gaussian density in $\mathbb{R}^d$.

The main object of inference is the marginal likelihood $p_\theta(y)$, obtained by integrating out the latent variables $z_0, \ldots, z_k$ in (2). This integration is typically intractable, so instead one works with the so-called evidence lower bound. Typically, this bound is derived using Jensen’s inequality (see, e.g., [Blei et al., 2017]); for our purposes, though, it will be convenient to derive it from the well-known Gibbs variational principle [Dupuis and Ellis, 1997]. For any Borel probability measure $\mu$ on $\Omega := (\mathbb{R}^d)^{k+1}$ and any measurable real-valued function $F : \Omega \to \mathbb{R}$,  
\[ -\log E_\mu[e^{-F(Z_0, \ldots, Z_k)}] = \inf_{\nu \in \mathcal{P}(\Omega)} \{ D(\nu \| \mu) + E_\nu[F(Z_0, \ldots, Z_k)] \}, \quad (3) \]
where $D(\cdot \| \cdot)$ is the Kullback–Leibler divergence and the infimum is over all Borel probability measures $\nu$ on $\Omega$. If we let $\mu$ be the marginal distribution of $Z_0, \ldots, Z_k$ in (2) and apply (3) to the function $F_\theta(z_0, \ldots, z_k) := -\log p(y | f_\theta(z_0, \ldots, z_k))$, we obtain the well-known variational formula  
\[ -\log p_\theta(y) = -\log \int p(y | f_\theta(z_0, \ldots, z_k)) \phi_d(z_0) \cdots \phi_d(z_k) \, dz_0 \cdots dz_k \]
\[ = \inf_{\nu \in \mathcal{P}(\Omega)} \{ D(\nu \| \mu) - \int_{\Omega} \log p(y | f_\theta(z_0, \ldots, z_k)) \nu(dz_0, \ldots, dz_k) \}, \quad (4) \]
The infimum in (4) is attained by the posterior density $p_\theta(z_0, \ldots, z_k | y)$ whose computation is also generally intractable, so one typically picks a suitable family $\nu_\beta(dz_0, \ldots, dz_k | y) = q_\beta(z_0, \ldots, z_k | y) dz_0 \cdots dz_k$ of approximate posteriors to obtain the variational upper bound  
\[ -\log p_\theta(y) \leq \inf_{\beta} F_{\theta, \beta}(y), \]
where $F_{\theta, \beta}(y) := D(\nu_\beta(\cdot | y) \| \mu) - \int_{\Omega} \log p(y | f_\theta(z_0, \ldots, z_k)) \nu_\beta(dz_0, \ldots, dz_k | y). \quad (5) \]

The choice of $q_\beta(\cdot | y)$ is driven by considerations of computational tractability vs. representational richness. A widely used family of approximate posteriors is given by the mean-field approximation: $q_\beta(\cdot | y)$ is the product of $k + 1$ Gaussian densities whose means $\tilde{b}_i(y), \ldots, \tilde{b}_k(y)$ and covariance matrices $C_0(y), \ldots, C_k(y)$ are also chosen from some parametric class of nonlinearities, and $\beta$ is then the collection of all the parameters of these transformations. The resulting inference procedure, known as stochastic backpropagation [Kingma and Welling, 2014; Rezende et al., 2014], involves estimating the gradients of the variational free energy $F_{\theta, \beta}(y)$ with respect to $\theta$ and $\beta$. This procedure hinges on two key steps:

**Reparametrization:** The joint law of $\tilde{b}_i(y) + C_i^{1/2}(y)Z_i$, $i \in \{0, \ldots, k\}$ with $Z_i \overset{i.i.d.}{\sim} \mathcal{N}(0, I_{d})$ is equal to the mean-field posterior $\nu_\beta(\cdot | y)$. Thus, we can express the variational free energy as  
\[ F_{\theta, \beta}(y) = \sum_{i=0}^{k} D(\mathcal{N}(\tilde{b}_i(y), C_0(y)) \| \mathcal{N}(0, I_d)) + E \left[ F_\theta(\tilde{b}_0(y) + C_0(y)^{1/2}Z_0, \ldots, \tilde{b}_k(y) + C_k(y)^{1/2}Z_0) \right]. \quad (6) \]

**Backpropagation with Monte Carlo:** Since the expectation in (6) is w.r.t. to a collection of i.i.d. standard Gaussian vectors, it follows that the gradients can be computed by interchanging differentiation and expectation and using automatic differentiation (backpropagation). Unbiased estimates of $\nabla_\star F_{\theta, \beta}(y), \star \in \{\theta, \beta\}$, can then be obtained by Monte Carlo sampling.

### 3 Neural Stochastic Differential Equations as DLGMs in the diffusion limit

In this work, we consider the continuous-time limit of (1), in analogy to the neural ODE framework of [Chen et al., 2018b] (which corresponds to the deterministic case $\sigma_i \equiv 0$). In this limit, the latent
object becomes a d-dimensional diffusion process \( X = \{ X_t \}_{t \in [0, 1]} \) given by the solution of the Itô stochastic differential equation (SDE)

\[
dX_t = b(X_t, t) \, dt + \sigma(X_t, t) \, dW_t, \quad t \in [0, 1]
\]

where \( W \) is the standard d-dimensional Wiener process or Brownian motion (see, e.g., [Bichteler 2002] or [Protter 2005] for background on diffusion processes and SDEs). The observed variable \( Y \) is generated conditionally on \( X_1 \): \( Y \sim p(\cdot|X_1) \). We focus on the case when both the drift \( b : \mathbb{R}^d \times [0, 1] \to \mathbb{R}^d \) and the diffusion coefficient \( \sigma : \mathbb{R}^d \times [0, 1] \to \mathbb{R}^{d \times d} \) are implemented by feedforward neural nets, and will thus use the term neural SDE to refer to (7).

The special case of (7) with \( X_0 = 0 \) and \( \sigma = I_d \) was studied by [Tzen and Raginsky 2019], who showed that generative models of this kind are sufficiently expressive. In particular, they showed that one can use a neural net drift \( b(\cdot, \cdot) \) and \( \sigma = I_n \) in (7) to obtain approximate samples from any target distribution for \( X_1 \) whose Radon–Nikodym derivative \( f \) w.r.t. the standard Gaussian measure on \( \mathbb{R}^d \) can be represented efficiently using neural nets. Moreover, only a polynomial overhead is incurred in constructing \( b \) compared to the neural net representing \( f \).

The main idea of the construction of [Tzen and Raginsky 2019] can be informally described as follows. Consider a target density of the form \( q(x) = f(x) \phi_d(x) \) for a sufficiently smooth \( f : \mathbb{R}^d \to \mathbb{R}_+ \) and the Itô SDE

\[
dX_t = \frac{\partial}{\partial x} \log Q_{1-t} f(X_t) \, dt + dW_t, \quad X_0 = 0; \quad t \in [0, 1]
\]

where \( Q_{1-t} f(x) := \mathbb{E}_{Z \sim \phi_d}[f(x + \sqrt{1-t} Z)] \). Then \( X_1 \sim q \), i.e., one can use (8) to obtain an exact sample from \( q \), and this construction is information-theoretically optimal (see, e.g., [Dar Pra 1991], [Lehec 2013, Eldan and Lee 2018], or [Tzen and Raginsky 2019]). The drift term in (8) is known as the Föllmer drift [Föllmer 1985]. Replacing \( Q_{1-t} f(x) \) by a Monte Carlo estimate and \( f(\cdot) \) by a suitable neural net approximation \( \hat{f}(\cdot; \theta) \), we can approximate the Föllmer drift by functions of the form

\[
\hat{b}(x, t; \theta) = \frac{\partial}{\partial x} \log \left\{ \frac{1}{N} \sum_{n=1}^{N} \hat{f}(x + \sqrt{1-t} z_n; \theta) \right\} = \frac{\sum_{n=1}^{N} \frac{\partial}{\partial x} \hat{f}(x + \sqrt{1-t} z_n; \theta)}{\sum_{n=1}^{N} \hat{f}(x + \sqrt{1-t} z_n; \theta)}.
\]

This has the following implications (see [Tzen and Raginsky 2019] for a detailed analysis):

- the complexity of representing the Föllmer drift by a neural net is comparable to the complexity of representing the Radon–Nikodym derivative \( f = \frac{dQ}{dp} \) by a neural net;
- the neural net approximation to the Föllmer drift takes both the space variable \( x \) and the time variable \( t \) as inputs, and its weight parameters \( \theta \) do not explicitly depend on time.

In some cases, this can be confirmed by direct computation. As an example, consider a stochastic deep linear neural net [Hardt and Ma 2017] in the diffusion limit:

\[
dX_t = A_t X_t \, dt + C_t \, dW_t, \quad X_0 = x_0; \quad t \in [0, 1].
\]

In this representation, the net is parametrized by the matrix-valued paths \( \{ A_t \}_{t \in [0, 1]} \) and \( \{ C_t \}_{t \in [0, 1]} \), and optimizing over the model parameters is difficult even in the deterministic case. On the other hand, the process \( X \) in (9) is Gaussian (in fact, all Gaussian diffusion processes are of this form), and the probability law of \( X_1 \) can be computed in closed form [Fleming and Rishel 1975, Chap. V, Sec. 9]: \( X_1 \sim \mathcal{N}(m, \Sigma) \) with

\[
m = \Phi_{0,1} x_0 \quad \text{and} \quad \Sigma = \int_0^1 \Phi_{t,1} C_t C_t^\top \Phi_{t,1}^\top \, dt,
\]

where \( \Phi_{s,t} \) (for \( s < t \)) is the fundamental matrix that solves the ODE

\[
\frac{d}{dt} \Phi_{s,t} = A_t \Phi_{s,t}, \quad \Phi_{s} = I_d; \quad t > s
\]

The Föllmer drift provides a more parsimonious representation that does not involve time-varying network parameters. Indeed, since \( q \) is the d-dimensional Gaussian density with mean \( m \) and covariance matrix \( \Sigma \), we have

\[
f(x) = e \exp \left\{ -\frac{1}{2} (x - m)^\top \Sigma^{-1} (x - m) + x^\top x \right\},
\]

4
where $c$ is a normalization constant. If $\det \Sigma \neq 0$, a straightforward but tedious computation yields

$$Q_t f(x) = c_t \exp \left\{ \frac{1}{2} \left( (x-m)\Sigma^{-1} (x-m) + x^\top x \right) \right\},$$

where $c_t > 0$ is a constant that does not depend on $x$, $v = (\Sigma^{-1} - I_d) x - \Sigma^{-1} m$, and $\mu_t = ((1-t) I_d + t \Sigma^{-1})^{-1}$. Consequently, the Föllmer drift is given by

$$\frac{\partial}{\partial x} \log Q_{t-t} f(x) = [(1-t)(\Sigma^{-1} - I_d)\Sigma_{1-t}(\Sigma^{-1} - I_d) - (\Sigma^{-1} - I_d)]x$$

$$- [(1-t)(\Sigma^{-1} - I_d)\Sigma_{1-t}(\Sigma^{-1} - \Sigma^{-1})m],$$

which is an affine function of $x$ with time-invariant parameters $\Sigma^{-1}$ and $m$.

## 4 Variational inference with neural SDEs

Our objective here is to develop a variational inference framework for neural SDEs that would leverage their expressiveness and the availability of adaptive black-box solvers for SDEs [Ilie et al., 2015]. We start by showing that all the building blocks of DLGMs described in Section 2 have their natural counterparts in the context of neural SDEs.

**Brownian motion as the latent object:** In the case of DLGMs, it was expedient to push all the randomness in the latent space $\Omega = (\mathbb{R}^d)^{k+1}$ into the i.i.d. standard Gaussians $Z_0, \ldots, Z_k$. An analogous procedure can be carried out for neural SDEs as well, except now the latent space is $\mathcal{W} = C([0,1]; \mathbb{R}^d)$, the space of continuous paths $\omega : [0,1] \rightarrow \mathbb{R}^d$, and the primitive random object is the Wiener process $W = \{W_t\}_{t \in [0,1]}$. The continuous-time analogue of the independence structure of the $Z_i$’s is the independent Gaussian increment property of $W$: for any $0 \leq s < t \leq 1$, the increment $W_t - W_s \sim \mathcal{N}(0,(t-s)I_d)$ is independent of $\{W_r : 0 \leq r \leq s\}$. Moreover, there is a unique probability law $\mu$ on $\mathcal{W}$ (the Wiener measure), such that, under $\mu$, $W_0 = 0$ almost surely and, for any $0 < t_1 < t_2 < \ldots < t_m \leq 1$, $W_{t_m} - W_{t_{m-1}}$ with $t_0 = 0$ are independent centered Gaussian random vectors with covariance matrices $(t_i - t_{i-1})I_d$.

Let us explicitly parametrize the drift and the diffusion in (7) as $b(x,t;\theta)$ and $\sigma(x,t;\theta)$, respectively. If, for each $\theta$, $b$ and $\sigma$ in (7) are Lipschitz-continuous in $x$ uniformly in $t \in [0,1]$, then there exists a mapping $f_\theta : \mathcal{W} \rightarrow \mathcal{W}$, such that $X = f_\theta(W)$, and this mapping is progressively measurable [Bichteler, 2002, Sec. 5.2]: If we denote by $[f_\theta(W)]_s$ the value of $f_\theta(W)$ at $t$, then

$$[f_\theta(W)]_s = \int_0^s b([f_\theta(W)]_r , s; \theta) \, ds + \int_0^s \sigma([f_\theta(W)]_r , s; \theta) \, dW_r,$$

that is, for each $t$, the path $\{[f_\theta(W)]_s \}_{s \in [0,1]}$ depends only on $\{W_s \}_{s \in [0,1]}$. With these ingredients in place, we have the following path-space analogue of (6):

$$P_\theta(dy, dw) = p(y|[f_\theta(w)]_1)\mu(dw) dy.$$

As before, the quantity of interest is the marginal density $p_\theta(y) := \int_{\mathbb{R}^d} p(y|[f_\theta(w)]_1)\mu(dw)$.

**The variational representation and Girsanov reparametrization:** The Gibbs variational principle also holds for measurable measures and measurable real-valued functions on the path space $\mathcal{W}$ [Boué and Dupuis, 1998], so we obtain the following variational formula:

$$- \log p_\theta(y) = \inf_{\nu \in \mathcal{P}(\mathcal{W})} \left\{ D(\nu || \mu) - \int_{\mathbb{R}^d} \log p(y|[f_\theta(w)]_1) \nu(dw) \right\}.$$

This formula looks forbidding, as it involves integration with respect to probability measures $\nu$ on path space $\mathcal{W}$. However, a significant simplification comes about from the fundamental result known as Girsanov’s theorem [Bichteler, 2002, Prop. 3.9.13]: any probability measure $\nu$ on $\mathcal{W}$ which is absolutely continuous w.r.t. the Wiener measure $\mu$ corresponds to the addition of a drift term to the basic Wiener process $W$. That is, there is a one-to-one correspondence between $\nu \in \mathcal{P}(\mathcal{W})$ with $D(\nu || \mu) < \infty$ and $\mathbb{R}^d$-valued random processes $u = \{u_t\}_{t \in [0,1]}$, such that each $u_t$ is measurable w.r.t. $\{W_s : 0 \leq s \leq t\}$ and $\mathbb{E}_\mu \left[ \frac{1}{2} \int_0^1 \|u_t\|^2 dt \right] < \infty$. Specifically, if we consider the Itô process

$$Z_t = \int_0^t u_s \, ds + W_t, \quad t \in [0,1],$$

then $Z_t$ is a $\mathcal{W}$-valued process with respect to $\mu$. This allows us to rewrite the variational formula as:

$$- \log p_\theta(y) = \inf_{\nu \in \mathcal{P}(\mathcal{W})} \left\{ D(\nu || \mu) - \int_{\mathbb{R}^d} \log p(y|[f_\theta(w)]_1) \nu(dw) \right\}.$$
then \( Z = \{ Z_t \}_{t \in [0,1]} \sim \nu \) with \( D(\nu \| \mu) = E_{\mu} \left[ \frac{1}{2} \| u_t \|^2 \, dt \right] \), and any such \( \nu \) can be realized in this fashion. This leads to the Girsanov reparametrization of the variational formula (12):

\[
- \log p_\theta(y) = \inf_u \mathbb{E}_\mu \left\{ \frac{1}{2} \int_0^1 \| u_t \|^2 \, dt + F_\theta \left( W + \int_0^t u_s \, ds \right) \right\},
\]

(14)

where \( W + \int_0^t u_s \, ds \) is shorthand for the process \( \{ W_t + \int_0^t u_s \, ds \}_{t \in [0,1]} \), and \( F_\theta(w) := -\log p(y | \{ f_\theta(w) \}_t) \).

**Mean-field approximation:** The next order of business is to develop a path-space analogue of the mean-field approximation. This is rather simple: we consider deterministic drifts of the form \( u_t = \tilde{b}(y, t; \beta) \), \( t \in [0,1] \), where \( \tilde{b}(t, y; \beta) \) is a neural net with weight parameters \( \beta \), such that \( \int_0^1 \| \tilde{b}(y, t; \beta) \|^2 \, dt < \infty \). The resulting process (13) is Gaussian and has independent increments with \( Z_t - Z_s \sim \mathcal{N}(\int_s^t \tilde{b}(y, s'; \beta) \, ds', (t-s) I_n) \), and we have the mean-field variational bound

\[
- \log p_\theta(y) \leq \inf_{\theta, \beta} \left\{ \frac{1}{2} \int_0^1 \| \tilde{b}(y, t; \beta) \|^2 \, dt + \mathbb{E}_\theta \left[ F_\theta \left( W + \int_0^t \tilde{b}(y, s; \beta) \, ds \right) \right] \right\}.
\]

(15)

One key difference from the DLGM set-up is worth mentioning: here, the only degree of freedom we need is an additive drift that affects the mean, whereas in the DLGM case we optimize over both the mean and the covariance matrix in Eq. (6).

## 5 Stochastic backpropagation in Wiener space

We are now faced with the problem of computing the gradients of the variational free energy

\[
F_{\theta, \beta}(y) := \frac{1}{2} \int_0^1 \| \tilde{b}(y, t; \beta) \|^2 \, dt + \mathbb{E}_\mu \left[ F_\theta \left( W + \int_0^t \tilde{b}(y, s; \beta) \, ds \right) \right]
\]

(16)

with respect to \( \theta \) and \( \beta \). The gradients of the first (KL-divergence) term on the right-hand side (16) can be computed straightforwardly using automatic differentiation, so we turn to the second term. To that end, let us define, for every \( \theta, \beta \), the Itô process \( X^{\theta, \beta} \) by

\[
X^{\theta, \beta}_t := X_0 + \int_0^t \tilde{b}(X^{\theta, \beta}_s, s; \theta) \, ds + \int_0^t \sigma(X^{\theta, \beta}_s, s; \theta) \, dW_s, \quad t \in [0,1]
\]

(17)

which is simply the result of adding the deterministic drift term \( \tilde{b}(y, t; \beta) \, dt \) to the neural SDE (7). Then the second term on the right-hand side of (16) is equal to \( -\mathbb{E}[\log p(y | X^{\theta, \beta}_t)] \), and the gradients with respect to \( \theta \) or \( \beta \) can be computed using chain rule and automatic differentiation, provided we have a way of differentiating the Itô process (17) w.r.t. these parameters (Gobet and Munos 2005). Formally, the Jacobians of the second term w.r.t. the parameters are given by

\[
\frac{\partial}{\partial \beta} \mathbb{E}[\log p(y | X^{\theta, \beta}_t)] = \mathbb{E} \left[ \frac{\partial}{\partial \beta} \log p(y | X^{\theta, \beta}_1) \frac{\partial X^{\theta, \beta}_t}{\partial \beta} \right],
\]

\[
\frac{\partial}{\partial \theta} \mathbb{E}[\log p(y | X^{\theta, \beta}_t)] = \mathbb{E} \left[ \frac{\partial}{\partial \theta} \log p(y | X^{\theta, \beta}_1) \frac{\partial X^{\theta, \beta}_t}{\partial \theta} \right],
\]

assuming the function \( x \rightarrow \log p(y | x) \) is sufficiently well-behaved to permit interchange of differentiation and integration. The computation of the pathwise derivatives of \( X^{\theta, \beta} \) with respect to \( \theta \) or \( \beta \) can now be carried out using the theory of stochastic flows (Kunita 1984).

**Theorem 5.1.** Assume the following:

1. The drift \( b(x, t; \theta) \) and the diffusion matrix \( \sigma(x, t; \theta) \) are Lipschitz-continuous with Lipschitz-continuous Jacobians in \( x \) and \( \theta \), uniformly in \( t \in [0,1] \).

2. The drift \( \tilde{b}(y, t; \beta) \) is Lipschitz-continuous with Lipschitz-continuous Jacobian in \( \beta \), uniformly in \( t \in [0,1] \).
Then the pathwise derivatives of $X = X_{t}^{\theta, \beta}$ in $\theta$ and $\beta$ are given by the following Itô processes:

$$
\frac{\partial X_t}{\partial \beta^i} = \int_0^t \left( \frac{\partial b_s}{\partial x} \frac{\partial X_s}{\partial \beta^i} + \frac{\partial \tilde{b}_s}{\partial x} \frac{\partial X_s}{\partial \beta^i} \right) ds + \sum_{\ell=1}^d \int_0^t \left( \frac{\partial \sigma_{s,\ell}}{\partial x} \frac{\partial X_s}{\partial \beta^i} \right) dW^\ell_s \tag{18}
$$

and

$$
\frac{\partial X_t}{\partial \theta^j} = \int_0^t \left( \frac{\partial b_s}{\partial \theta^j} + \frac{\partial \tilde{b}_s}{\partial \theta^j} \right) ds + \sum_{\ell=1}^d \int_0^t \left( \frac{\partial \sigma_{s,\ell}}{\partial x} \frac{\partial X_s}{\partial \theta^j} \right) dW^\ell_s \tag{19}
$$

where, e.g., $b_s$ is shorthand for $b(X_s^{\theta, \beta}, s; \theta)$, $\sigma_{s, \ell}$ denotes the $\ell$th column of $\sigma(X_s^{\theta, \beta}, s; \theta)$, and $W^1, \ldots, W^d$ are the independent scalar coordinates of the $d$-dimensional Wiener process $W$.

**Proof.** We will use the results of Kunita [1984] on differentiability of the solutions of Itô SDEs w.r.t. initial conditions. Consider an $m$-dimensional Itô process of the form

$$
Z_t(\xi) = \xi + \int_0^t f_0(Z_s(\xi), s) ds + \sum_{i=1}^m \int_0^t f_i(Z_s(\xi), s) dW^i_s, \quad t \in [0, 1] \tag{20}
$$

where $W^1, \ldots, W^m$ are independent standard scalar Brownian motions, with the following assumptions:

1. The initial condition $Z_0(\xi) = \xi \in \mathbb{R}^m$.
2. The vector fields $f_j : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^m$, $j \in \{0, \ldots, m\}$, are globally Lipschitz-continuous and have Lipschitz-continuous gradients, uniformly in $t \in [0, 1]$.

Then Kunita [1984, Chap. 2, Thm. 3.1] the pathwise derivatives of $Z$ w.r.t. the initial condition $\xi$ exist and are given by the Itô processes

$$
\frac{\partial Z_t(\xi)}{\partial \xi^i} = e_i + \int_0^t \frac{\partial}{\partial \xi^i} f_0(Z_s(\xi), s) dZ_s(\xi) + \sum_{j=1}^m \int_0^t \frac{\partial}{\partial \xi^i} \sigma_j(Z_s(\xi), s) \frac{\partial Z_s(\xi)}{\partial \xi^j} dW^j_s, \tag{21}
$$

where $e_1, \ldots, e_m$ are the standard basis vectors in $\mathbb{R}^m$. Now suppose that $\beta \in \mathbb{R}^k$, $\theta \in \mathbb{R}^n$, let $m := d + k + n$, and define the vector fields $f_0(z, t)$ for $z = (x^T, \beta^T, \theta^T)^T \in \mathbb{R}^m$ and $t \in [0, 1]$ by

$$
f_0(z, t) := \left( \begin{array}{c} b(x, t; \beta) + \tilde{b}(y, t; \beta) \\ 0 \end{array} \right) \quad \text{and} \quad f_j(z, t) := \left( \begin{array}{c} \sigma_j(x, t; \beta) \cdot 1_{j \in \{1, \ldots, d\}} \\ 0 \end{array} \right), \tag{22}
$$

where $\sigma_j(x, t; \beta)$ is the $j$th column of $\sigma(x, t; \beta)$. These vector fields satisfy the above Lipschitz continuity condition by hypothesis. Consider the Itô process (20) with the initial condition $\xi = (0^T, \beta^T, \theta^T)^T$. Then evidently

$$
Z_t(\xi) = \left( \begin{array}{c} X_{t}^{\theta, \beta} \\ \beta \\ \theta \end{array} \right), \quad t \in [0, 1]
$$

and Eqs. (18) and (19) follow from (21), (22), and the chain rule of multivariable calculus. □

From the above, it follows that we can perform variational inference with neural SDEs using the following two ingredients:

1. A black-box SDE solver: For a given initial condition $z \in \mathbb{R}^m$, initial and final times $0 \leq t_0 < t_1 \leq 1$, drift $f : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^m$, and diffusion coefficient matrix $g : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^{m \times d}$, we will denote by SDE.Solve$(z, t_0, t_1, f, g)$ the output of any black-box procedure that computes or approximates the solution at time $t_1$ of the Itô SDE

$$
dZ_t = f(Z_t, t) dt + g(Z_t, t) dW_t, \quad t \in [t_0, t_1], \quad \text{with} \quad Z_{t_0} = z.
$$

The solver could be as simple as a vanilla Euler–Maruyama scheme or as complex as an adaptive time-stepping algorithm with strong approximation guarantees [The et al., 2013].
We use \( (23) \) parametrized by \( \sigma \) and \( \beta \), and the pathwise derivatives \( \frac{\partial X}{\partial \beta} \) and \( \frac{\partial X}{\partial \sigma} \) by a call to SDE. Solve with \( f \) and \( g \) consisting of \( b(\cdot; \theta) \), \( \sigma(\cdot; \theta) \), \( \tilde{b}(\cdot; \beta) \) and their Jacobians w.r.t. \( x \), \( \beta \), and \( \theta \).

The gradients of the free energy w.r.t. \( \beta \) and \( \theta \) can then be estimated using Monte Carlo methods, by averaging multiple independent runs of the SDE solver. It is worth mentioning that, in contrast to the neural ODE framework of \cite{Chen2018a}, where one has to augment the original ODE with the so-called adjoint ODE that has to be solved backwards in time to obtain the gradients w.r.t. the model parameters, here we run our SDE solver forwards in time.

6 Experimental results

We evaluated the performance of stochastic backpropagation using gradient descent on synthetic data. The code for all experiments was written Python using PyTorch and executed on a CPU. The synthetic data were generated via Euler discretization of the diffusion process

\[
dX_t = \text{sigmoid}(AX_t) \, dt + dW_t, \quad t \in [0, 1]
\]  

where \( \text{sigmoid}(\cdot) \) is the coordinatewise sigmoid (logistic) activation function. The observations \( Y_1, \ldots, Y_n \in \mathbb{R}^d \) were generated by sampling \( n \) independent copies of this process and then adding small independent Gaussian perturbations to each copy of \( X_t \). The variational approximations were generated by the Ornstein–Uhlenbeck process

\[
dX_t = BX_t \, dt + dW_t.
\]  

Note that the drift term in (24) depends on \( X_t \), so this is not a mean-field approximation. Nevertheless, variational approximations of the form \( dX_t = \tilde{b}(X_t; \beta) \, dt + dW_t \) are still valid since they satisfy the conditions of Girsanov’s theorem, and our framework can be easily extended to this case. One advantage of using the Ornstein–Uhlenbeck process is that it is a Gaussian process, whose mean and covariance matrix can be computed in closed form. The ground-truth parameter \( A \) and the initial data \( X_0 \) were randomly chosen with elements drawn i.i.d. from \( \mathcal{N}(0, 1) \); all other parameters were likewise randomly initialized.

We use (23) parametrized by \( A \in \mathbb{R}^{d \times d} \) as the neural SDE model, and take \( p(y|x) \) to be Gaussian with mean \( x \) and covariance matrix \( \sigma^2 I_d \), where the variance parameter \( \sigma^2 \) is larger than the variance of the noise used in generating \( Y_1, \ldots, Y_n \). This model misspecification introduced by higher variance in evaluating the posterior log-likelihood can be thought of as a form of regularization: \( \sigma^2 \) is tuned so that the posterior log-likelihood is of the same order of magnitude as that of the KL divergence w.r.t. the underlying Wiener process; in this way, they have similar contributions to the free energy, and optimization is more efficient.

For appropriate choices of parameters, performing vanilla gradient descent with constant step size leads to a decrease of the free energy: the log-likelihood of the data w.r.t. the learned generative parameters increases, while the KL divergence between the auxiliary drift (the variational approximation) and the underlying Wiener process decreases. As proof of concept, we show this for a low-dimensional ground-truth parameter \( A \in \mathbb{R}^{3 \times 3} \) (and thus the variational approximation matrix of the same dimensions), \( n = 10 \) samples, and 20 Euler discretization steps, with standard Monte Carlo sampling.

Figure 1 shows the decrease in total free energy over iterations, while Figure 2 shows the decrease in KL divergence between the variational approximation and the Wiener process; the divergence and log-likelihood terms are optimized at roughly the same rate. Figure 3 shows the decrease in mean squared error of the predictions w.r.t. training data; it does not converge to the empirical global minimum as a consequence of the nonconvexity of the objective function and the bias of the gradient estimators used, which merits further examination. On the other hand, Figure 4 shows a decline markedly similar to that of the training error, indicating that, despite the modest sample size and liberal discretization increments, the learned model generalizes well.
Figure 1: Free energy over GD iterations
Figure 2: KL divergence over GD iterations
Figure 3: MSE of training error over iterations (uniformly subsampled for 200 iterations)
Figure 4: Free energy for test data (uniformly subsampled for 200 iterations)

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