SBGM: Score-Based Generative Models in JAX.

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Summary

Statement of need

Diffusion-based generative models Ho et al. (2020) are a method for density estimation and sampling from high-dimensional distributions. A sub-class of these models, score-based diffusion generatives models (SBGMs, (Song, Sohl-Dickstein, et al., 2021)), permit exact-likelihood estimation via a change-of-variables associated with the forward diffusion process (Song, Durkan, et al., 2021). Diffusion models allow fitting generative models to high-dimensional data in a more efficient way than normalising flows since only one neural network model parameterises the diffusion process as opposed to a stack of networks in typical normalising flow architectures.

The software we present, `sbgm`, is designed to be used by researchers in machine learning and the natural sciences for fitting diffusion models with a suite of custom architectures for their tasks. These models can be fit easily with multi-accelerator training and inference within the code. Typical use cases for these kinds of generative models are emulator approaches (Spurio Mancini et al., 2022), simulation-based inference (likelihood-free inference, (Cranmer et al., 2020)), field-level inference (Andrews et al., 2023) and general inverse problems (Feng et al., 2023; Feng & Bouman, 2024; Song et al., 2022) (e.g. image inpainting (Song, Sohl-Dickstein, et al., 2021) and denoising (Chung et al., 2022; Daras et al., 2024)). This code allows for seamless integration of diffusion models to these applications by allowing for easy conditioning of data on parameters, classifying variables or other data such as images.

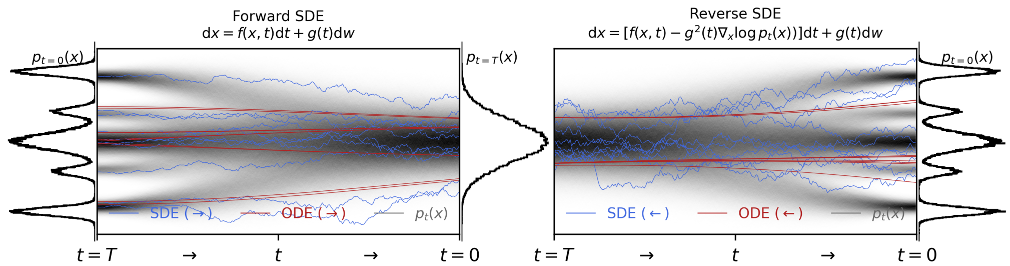

Figure 1: A diagram showing how to map data to a noise distribution (the prior) with an SDE, and reverse this SDE for generative modeling. One can also reverse the associated probability flow ODE, which yields a deterministic process that samples from the same distribution as the SDE. Both the reverse-time SDE and probability flow ODE can be obtained by estimating the score.

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Mathematics

Diffusion models model the reverse of a forward diffusion process on samples of data x by adding a sequence of noisy perturbations (Sohl-Dickstein et al., 2015).

Score-based diffusion models model the forward diffusion process with Stochastic Differential Equations (SDEs, (Song, Sohl-Dickstein, et al., 2021)) of the form

$$\text{d}x = f(x,t)\text{d}t + g(t)\text{d}w,$$

where $f(x,t)$ is a vector-valued function called the drift coefficient, $g(t)$ is the diffusion coefficient and $\text{d}w$ is a sample of infinitesimal noise. The solution of a SDE is a collection of continuous random variables describing a path parameterised by a 'time' variable t.

The SDE itself is formulated by design and existing options include the variance exploding (VE), variance preserving (VP) and sub-variance preserving (SubVP). These equations describe how the mean and covariances of the distributions of noise added to the data evolve with time.

the reverse of the SDE, mapping from multivariate Gaussian samples to data, is of the form

$$\text{d}x = [f(x,t) - g^2(t)\nabla_x \log p_t(x)]\text{d}t + g(t)\text{d}w,$$

where the score function $\nabla_x \log p_t(x)$ is substituted with a neural network $s_\theta(x(t),t)$ for the sampling process. This network predicts the noise added to the image at time t with the forward diffusion process, in accordance with the SDE, and removes it. This defines the sampling chain for a diffusion model.

The score-based diffusion model for the data is fit by optimising the parameters of the network θ via stochastic gradient descent of the score-matching loss

where $\lambda(t)$ is an arbitrary scalar weighting function, chosen to preferentially weight certain times - usually near $t=0$ where the data has only a small amount of noise added. Here, $p_t(x(t)|x(0))$ is the transition kernel for Gaussian diffusion paths. This is defined depending on the form of the SDE (Song, Sohl-Dickstein, et al., 2021) and for the common variance-preserving (VP) SDE the kernel is written as

where $\mathcal{G}[\cdot]$ is a Gaussian distribution, $\mu_t = \exp(-\int_0^t \text{d}s\ \beta(s))$ and $\sigma_t^2 = 1 - \mu_t$. $\beta(t)$ is typically chosen to be a simple linear function of t.

In Figure 1 the forward and reverse diffusion processes are shown for a samples from a Gaussian mixture with their corresponding SDE and ODE paths.

The reverse SDE may be solved with Euler-Murayama sampling (or other annealed Langevin sampling methods) which is featured in the code.

However, many of the applications of generative models depend on being able to calculate the likelihood of data. In [1] it is shown that any SDE may be converted into an ordinary differential equation (ODE) without changing the distributions, defined by the SDE, from which the noise is sampled from in the diffusion process. This ODE is known as the probability flow ODE and is written

$$\text{d}x = [f(x,t) - g^2(t)\nabla_x \log p_t(x)]\text{d}t = f'(x,t)\text{d}t.$$

This ODE can be solved with an initial-value problem that maps a prior sample from a multivariate Gaussian to the data distribution. This inherits the formalism of continuous normalising flows (Chen et al., 2019; Grathwohl et al., 2018) without the expensive ODE simulations used to train these flows.

The likelihood estimate under a score-based diffusion model is estimated by solving the change-of-variables equation for continuous normalising flows.

$$\frac{\partial}{\partial t}\log p(x(t)) = \nabla_x \cdot f(x(t), t),$$

which gives the log-likelihood of a single datapoint $x(0)$ as

$$\log p(x(0)) = \log p(x(T)) + \int_{t=0}^{t=T} \text{d}t \; \nabla_x \cdot f(x, t).$$

The code implements these calculations also for the Hutchinson trace estimation method (Grathwohl et al., 2018) that reduces the computational expense of the estimate.

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