Bayesian Inference and Information based model check of Langevin Systems

Sabarno Saha ¹ Dr. Rajesh Singh ² November 13, 2024

¹Department of Physical Sciences IISERK

²Department of Physical Sciences IIT Madras

Introduction

1. Stochastic Thermodynamics

- Stochastic Processes
- · Brownian Motion
- Stochastic Differential equation
- Stochastic Integrals
- Langevin Equation
- Fokker-Planck Equation
- · Euler-Maruyuma Integrator

2. Bayesian Inference

- · Bayes Theorem
- Prior Assignment
- Example

Introduction(Contd.)

- 4. Information Theory
 - · Shannon Information
 - Fisher Information
 - Kullback Liebler Divergence
- 5. Nested Sampling
 - · Likelihood Function
 - MCMC
 - · Evidence Calculation
- 6. Model Check
 - · Information check
 - Scaling of Steps
 - p-value check

Stochastic Thermodynamics

Definition

A stochastic process is a sequence of random variables where the indexing of the variables often carries the notion of time.

For example, we have Brownian motion, which is represented using the Wiener process (a stochastic process).

Definition

A Wiener process \hat{W} is a stochastic process which has the following conditional pdf

$$P(\hat{W}(t + \Delta t) = x | \hat{W}(t) = x') = \frac{1}{\sqrt{2\pi\Delta t}} \exp\left(-\frac{(x - x')^2}{2\Delta t}\right)$$

The initial conditions are $P(\hat{W}(0) = x) = \delta(x)$ where $\delta(x)$ is the Dirac Delta function.

Stochastic Thermodynamics : Wiener Process

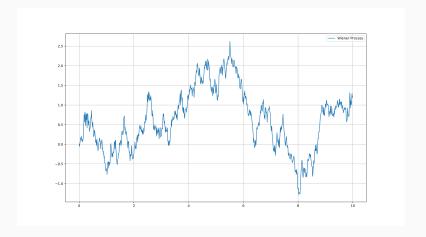


Figure 1: Wiener Process

Stochastic Thermodyamics: Noise

Definition

The White Gaussian noise $\hat{\xi}(x)$ is defined as

$$\lim_{\Delta t \to 0} \frac{\hat{W}(t + \Delta t) - \hat{W}(t)}{\Delta t}$$

Definition

The White Gaussian noise $\hat{\xi}(x)$ is also defined as any random variable that has the following properties

- $\cdot \mathbb{E}_t[\hat{\xi}(t)] = 0$
- $\mathbb{E}_t[\hat{\xi}(t')\hat{\xi}(t)] \propto \delta(t-t')$

We can have other types of noise as well like telegraphic noise, which we'll see briefly at the very end.

Stochastic Thermodynamics: SDE

Definition

A stochastic differential equation is an equation of the form

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = a(\hat{x}, t) + b(\hat{x}, t) \circ \hat{\zeta}(x)$$

where $\hat{\zeta}(t)$ is some form of stochastic noise and \circ is the type of product rule being used.

The two most common type of product rules are the Ito and the Stratonovich product rules. We are not going to discuss on this further.

7

Stochastic Thermodynamics: Langevin Equation

This is type of equation provides a nice way to model SDE, named after Paul Langevin(also known for his contributions towards the twin paradox). The Langevin equation is basically Newton's second law of motion but with an added noise term.

Definition

A Langevin Equation is an equation of the form

$$m\frac{\mathrm{d}\hat{v}}{\mathrm{d}t} = a(\hat{x}, \hat{v}, t) + b(\hat{x}, \hat{v}, t) \circ \hat{\xi}(t)$$

where a and b are known functions.

Stochastic Thermodynamics: Fokker-Planck Equation

Definition (Fokker Planck Equation)Suppose we have the following langevin equation

$$m\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = a(\hat{x}, t) + b(\hat{x}, t)\hat{\zeta}(t) \tag{1}$$

where $\zeta(t)$ satisfies the following properties.

- $\cdot \mathbb{E}_t[\zeta(t)] = 0$
- $\cdot \mathbb{E}_t[\zeta(t)^2] = 1$

The corresponding Fokker-Planck is given as

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}(a(x,t)P(x,t)) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(b(x,t)^2P(x,t))$$
(2)

Stochastic Thermodynamics : Euler-Maruyama Integrator

Definition (EM Integrator)

To simulate Stochastic processes, we use the Euler-Maruyama Integrator which is given as, which is just the discretized SDE,

$$\hat{x}(t+dt) = \hat{x}(t) + a(\hat{x},t)dt + b(\hat{x},t)\sqrt{dt}\hat{N}$$
(3)

where $\hat{N} \sim Normal(0,1)$

Bayesian Inference: Bayes' Theorem

Bayesian Inference: Prior Assignment

Bayesian Inference : Example

Information Theory: Shannon Information

Information Theory: Fisher Information

Information Theory: Kullback Liebler Divergence

Information Theory: Typical set of models

Information Theory: Jeffrey's prior

Nested Sampling : Likelihood

Nested Sampling : MCMC

Nested Sampling: Evidence

Nested Sampling : Error

Model Check

Model Check