

Machine Learning with Signal Processing

Part II: Stochastic Differential Equations

Arno Solin

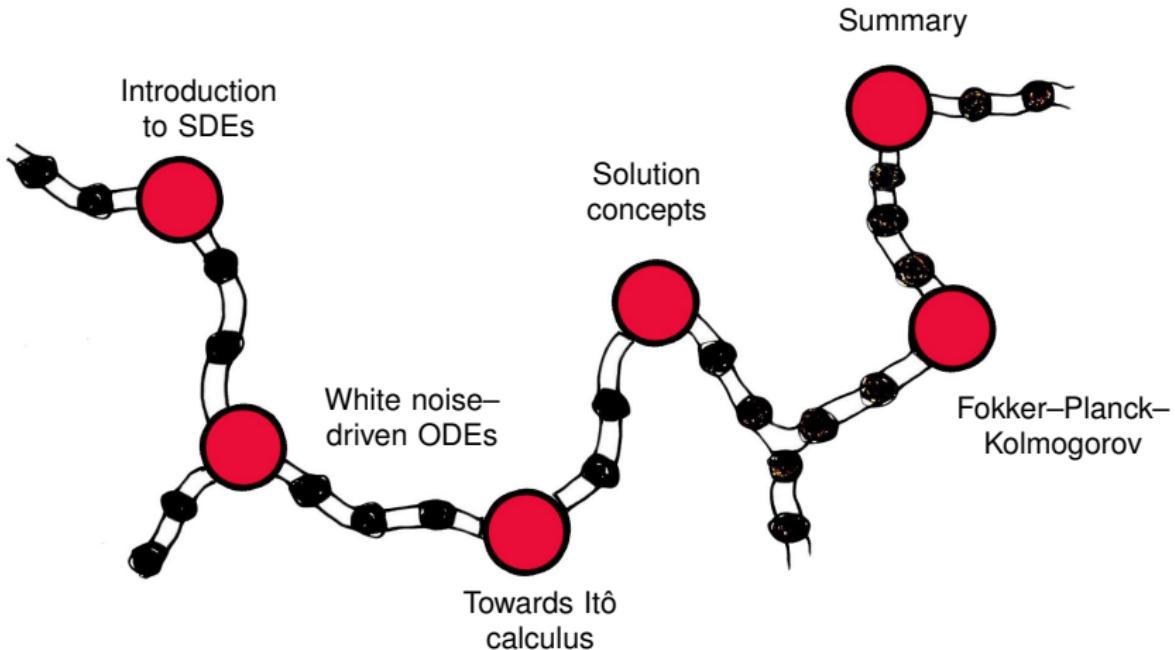
Assistant Professor in Machine Learning
Department of Computer Science
Aalto University

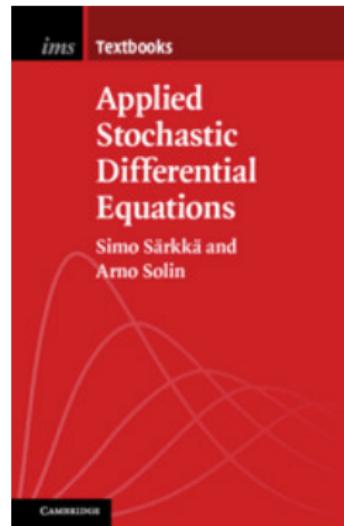
ICML 2020 TUTORIAL

 @arnosolin

 arno.solin.fi

Outline





- S. Särkkä and A. Solin (2019). **Applied Stochastic Differential Equations**. Cambridge University Press. Cambridge, UK.
Book PDF and codes for replicating examples available online.

Differential equations model how things change

- ▶ Ordinary differential equations (ODEs)
(deterministic)
- ▶ Stochastic differential equations (SDEs)
(stochastic)

What is a stochastic differential equation (SDE)?

- ▶ Consider an ordinary differential equation (ODE):

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t)$$

- ▶ Then we add white noise to the right hand side:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) + \mathbf{L}(\mathbf{x}, t) \mathbf{w}(t)$$

- ▶ $\mathbf{f}(\mathbf{x}, t)$ is the drift function and $\mathbf{L}(\mathbf{x}, t)$ is the dispersion matrix (diffusion term)
- ▶ Now we have a stochastic differential equation (SDE)

White noise

1. $\mathbf{w}(t_1)$ and $\mathbf{w}(t_2)$ are independent if $t_1 \neq t_2$
2. $t \mapsto \mathbf{w}(t)$ is a Gaussian process with mean and covariance:

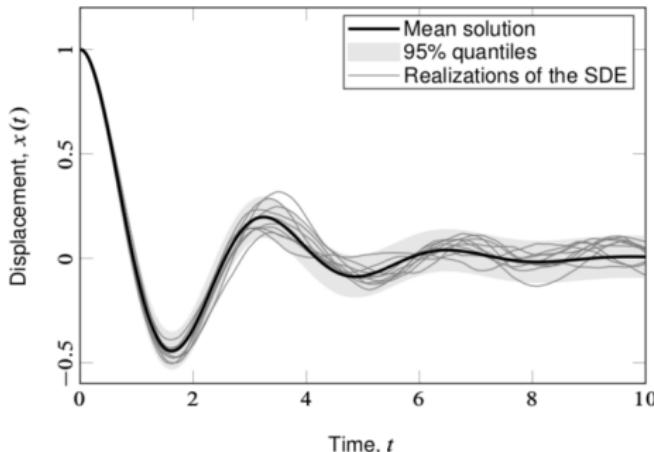
$$\mathbb{E}[\mathbf{w}(t)] = \mathbf{0},$$

$$\mathbb{E}[\mathbf{w}(t) \mathbf{w}^T(s)] = \delta(t - s) \mathbf{Q}$$



- ▶ \mathbf{Q} is the **spectral density** of the process
- ▶ The sample path $t \mapsto \mathbf{w}(t)$ is **discontinuous almost everywhere**
- ▶ White noise is **unbounded** and it takes arbitrarily large positive and negative values at any finite interval

What does a solution of an SDE look like?



Solution paths of a stochastic spring model

$$\frac{d^2x(t)}{dt^2} + \gamma \frac{dx(t)}{dt} + \nu^2 x(t) = w(t)$$

SDEs as white noise–driven differential equations

- ▶ Treating SDEs as white noise–driven differential equations has its limits

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) + \mathbf{L}(\mathbf{x}, t) \mathbf{w}(t)$$

- ▶ For linear equations the approach works
- ▶ But this interpretation breaks down in the general setting:
 - ▶ The chain rule of calculus starts giving wrong answers!
 - ▶ With non-linear differential equations the behaviour becomes unexpected
 - ▶ Trying to prove the existence of solutions becomes tricky
- ▶ The source of all the problems is the everywhere discontinuous white noise $\mathbf{w}(t)$
- ▶ So how should we really formulate SDEs?

Equivalent integral equation

- We have a **differential equation** of the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) + \mathbf{L}(\mathbf{x}, t) \mathbf{w}(t)$$

- **Integrating** the differential equation from t_0 to t gives:

$$\mathbf{x}(t) - \mathbf{x}(t_0) = \int_{t_0}^t \mathbf{f}(\mathbf{x}(t), t) dt + \int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) \mathbf{w}(t) dt$$

- The **first integral** is just a **Riemann/Lebesgue integral**
- The **second integral** is the problematic one due to the **white noise** (this is the interesting part!)

Attempt 1: Riemann integral

- ▶ In the **Riemannian sense** the integral would be defined as

$$\int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) \mathbf{w}(t) dt = \lim_{n \rightarrow \infty} \sum_k \mathbf{L}(\mathbf{x}(t_k^*), t_k^*) \mathbf{w}(t_k^*) (t_{k+1} - t_k),$$

where $t_0 < t_1 < \dots < t_n = t$ and $t_k^* \in [t_k, t_{k+1}]$

- ▶ **Upper and lower sums** are defined as the selections of t_k^* such that the integrand $\mathbf{L}(\mathbf{x}(t_k^*), t_k^*) \mathbf{w}(t_k^*)$ has its maximum and minimum values, respectively
- ▶ The Riemann integral exists if the **upper and lower sums** converge to the **same value**
- ! Because white noise is **discontinuous everywhere**, the Riemann integral **does not exist**

Attempt 2: Stieltjes integral [1/2]

- ▶ A Stieltjes integral is more general and allows for discontinuous integrands
- ▶ We can interpret the increment $\mathbf{w}(t) dt$ as increments of another process $\beta(t)$ such that

$$\int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) \mathbf{w}(t) dt = \int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) d\beta(t).$$

- ▶ It turns out that a suitable process for this purpose is Brownian motion...

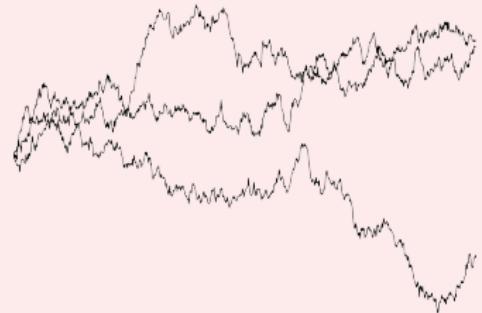
Brownian motion

1. Gaussian increments:

$$\Delta\beta_k \sim N(\mathbf{0}, \mathbf{Q} \Delta t_k),$$

where $\Delta\beta_k = \beta(t_{k+1}) - \beta(t_k)$
and $\Delta t_k = t_{k+1} - t_k$

2. Non-overlapping increments are independent



- ▶ **Q** is the **diffusion matrix** of the Brownian motion.
- ▶ Brownian motion $t \mapsto \beta(t)$ has **discontinuous derivative everywhere**
- ▶ **White noise** can be considered the formal **derivative of Brownian motion**
 $w(t) = d\beta(t)/dt$

Attempt 2: Stieltjes integral [2/2]

- ▶ Stieltjes integral is defined as a limit of the form

$$\int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) d\beta = \lim_{n \rightarrow \infty} \sum_k \mathbf{L}(\mathbf{x}(t_k^*), t_k^*) [\beta(t_{k+1}) - \beta(t_k)],$$

where $t_0 < t_1 < \dots < t_n$ and $t_k^* \in [t_k, t_{k+1}]$

- ▶ The limit t_k^* should be independent of the position on the interval $t_k^* \in [t_k, t_{k+1}]$
- ▶ For integration with respect to Brownian motion this is not the case

! Thus, the Stieltjes integral definition does not work either

Attempt 3: Lebesgue integral

- ▶ In a Lebesgue integral we could interpret $\beta(t)$ to define a 'stochastic measure'
- ▶ Essentially, this will also lead to the definition

$$\int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) d\beta = \lim_{n \rightarrow \infty} \sum_k \mathbf{L}(\mathbf{x}(t_k^*), t_k^*) [\beta(t_{k+1}) - \beta(t_k)],$$

where $t_0 < t_1 < \dots < t_n$ and $t_k^* \in [t_k, t_{k+1}]$.

- ▶ Again, the limit should be independent of the choice $t_k^* \in [t_k, t_{k+1}]$
- ▶ Also our 'measure' is not really a sensible measure

! The Lebesgue integral **does not work either**

Attempt 4: Itô integral

- ▶ The solution to the problem is the Itô stochastic integral
- ▶ The idea is to fix the choice to $t_k^* = t_k$, and define the integral as

$$\int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) d\beta(t) = \lim_{n \rightarrow \infty} \sum_k \mathbf{L}(\mathbf{x}(t_k), t_k) [\beta(t_{k+1}) - \beta(t_k)]$$

- ▶ This Itô stochastic integral turns out to be a sensible definition of the integral
- ▶ However, the resulting integral does not obey the computational rules of ordinary calculus
- ▶ Instead of ordinary calculus we have Itô calculus

Itô stochastic differential equations

- ▶ Consider the white noise–driven ODE

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) + \mathbf{L}(\mathbf{x}, t) \mathbf{w}(t)$$

- ▶ This is actually defined as the Itô integral equation

$$\mathbf{x}(t) - \mathbf{x}(t_0) = \int_{t_0}^t \mathbf{f}(\mathbf{x}(t), t) dt + \int_{t_0}^t \mathbf{L}(\mathbf{x}(t), t) d\beta(t),$$

which should be true for arbitrary t_0 and t

- ▶ Which can be written (considering the limits ‘small’) as

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t) dt + \mathbf{L}(\mathbf{x}, t) d\beta$$

- ▶ This is the canonical form of an Itô SDE

Connection with white noise–driven ODEs

- ▶ Let's formally divide by dt , which gives

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) + \mathbf{L}(\mathbf{x}, t) \frac{d\beta}{dt}$$

- ▶ Thus we can interpret $d\beta/dt$ as white noise \mathbf{w} (not an entity as such, only the formal derivative)
- ▶ Note that we cannot define more general equations

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(\mathbf{x}(t), \mathbf{w}(t), t),$$

because we cannot re-interpret this as an Itô integral equation

Non-linear SDEs

- ▶ There is no general solution method for **non-linear SDEs**

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t) dt + \mathbf{L}(\mathbf{x}, t) d\beta$$

- ▶ However, **numerical simulation** of solution trajectories is usually possible (e.g., with stochastic Runge–Kutta)
- ▶ The simplest alternative is the **Euler–Maruyama method**:

$$\hat{\mathbf{x}}(t_{k+1}) = \hat{\mathbf{x}}(t_k) + \mathbf{f}(\hat{\mathbf{x}}(t_k), t_k) \Delta t + \mathbf{L}(\hat{\mathbf{x}}(t_k), t_k) \Delta \beta_k,$$

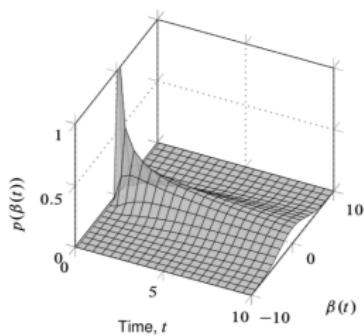
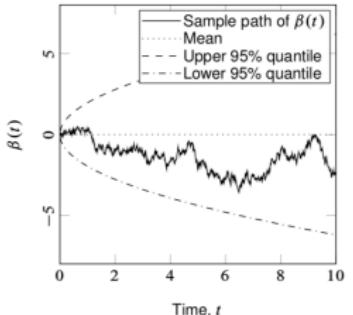
where $\Delta \beta_k \sim \mathcal{N}(\mathbf{0}, \mathbf{Q} \Delta t)$

Solution concepts in SDEs

- ▶ Path of a Brownian motion which is solution to stochastic differential equation

$$\frac{dx}{dt} = w(t)$$

- ▶ Strong vs. weak solutions
- ▶ Evolution of the probability density of the solution trajectories is given by the Fokker–Planck–Kolmogorov PDE



Fokker–Planck–Kolmogorov PDE

The probability density $p(\mathbf{x}, t)$ of the solution of the SDE

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t) dt + \mathbf{L}(\mathbf{x}, t) d\beta$$

solves the Fokker–Planck–Kolmogorov PDE

$$\begin{aligned}\frac{\partial p(\mathbf{x}, t)}{\partial t} = & - \sum_i \frac{\partial}{\partial x_i} [f_i(\mathbf{x}, t) p(\mathbf{x}, t)] \\ & + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \left\{ [\mathbf{L}(\mathbf{x}, t) \mathbf{Q} \mathbf{L}^\top(\mathbf{x}, t)]_{ij} p(\mathbf{x}, t) \right\}\end{aligned}$$

- ▶ In physics literature it is called the Fokker–Planck equation
- ▶ In stochastics it is the forward Kolmogorov equation

Summary

- ▶ Stochastic differential equations (SDE) can be seen as differential equations with a stochastic driving force
- ▶ SDEs are typical in **physics**, **engineering**, and **finance** applications
- ▶ A heuristic **white noise** formulation has problems with the **chain rule**, **non-linearities**, and **solution existence**
- ▶ Instead, use the **Itô stochastic integral** (calculus)
- ▶ Various **solution concepts**; in general, non-linear SDEs are tricky to solve (good schemes for simulation exist though)

3

- ▶ Three views into Gaussian processes
- ▶ (one of which is in terms of linear SDEs)

Bibliography

These references are sources for finding a more detailed overview on the topics of this part:

- S. Särkkä and A. Solin (2019). *Applied Stochastic Differential Equations*. Cambridge University Press. Cambridge, UK.
- B. Øksendal (2003). *Stochastic Differential Equations: An Introduction with Applications*. Springer, New York.
- P. E. Kloeden and E. Platen (1999). *Numerical Solution to Stochastic Differential Equations*. Springer, New York.