Diffusion processes

and the Fokker-Planck equation (some ideas...)

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- First-order stochastic systems driven by noise
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- Diffusion processes

3 Numerical simulations of SDE
- Stochastic modeling with SDE
- Numerical schemes

4 Stochastic Hamiltonian dynamical systems

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Linear or non linear dynamical systems

- Discrete linear dynamical system:

$$\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{D}\dot{\boldsymbol{q}} + \boldsymbol{K}\boldsymbol{q} = \boldsymbol{F}(t)\,,$$

or for $\boldsymbol{u} = (\boldsymbol{q}, \boldsymbol{p})$, $\boldsymbol{p} = \boldsymbol{M}\dot{\boldsymbol{q}}$:

$$\dot{\boldsymbol{u}}(t) = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{M}^{-1} \\ -\boldsymbol{K} & -\boldsymbol{D}\boldsymbol{M}^{-1} \end{bmatrix} \boldsymbol{u}(t) + \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{I} \end{bmatrix} \boldsymbol{F}(t)\,, \quad \boldsymbol{u}(0) = \boldsymbol{u}_0\,.$$

- Non-linear dynamical system, *e.g.* the Duffing oscillator:

$$M\ddot{q} + D\dot{q} + Kq + K_0 q^3 = F(t)\,,$$

or:

$$\dot{\boldsymbol{u}}(t) = \boldsymbol{b}(\boldsymbol{u}, t) + \boldsymbol{a}F(t)\,, \quad \boldsymbol{u}(0) = \boldsymbol{u}_0\,,$$

with $\boldsymbol{b}(\boldsymbol{u}, t) = \begin{pmatrix} M^{-1}p \\ -DM^{-1}p - Kq - K_0 q^3 \end{pmatrix}$, $\boldsymbol{a} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Example: free vibrations of a single oscillator

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$$\dot{\boldsymbol{U}}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q \\ M\dot{q} \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & M^{-1} \\ -K & -DM^{-1} \end{bmatrix}}_{-\boldsymbol{L}}\boldsymbol{U}(t)\,, \quad \boldsymbol{U}(0) = \boldsymbol{U}_0\,,$$

where $\boldsymbol{U}_0$ is a r.v. with *marginal PDF* $\pi_0(\boldsymbol{u}_0)$.

- Formally $\boldsymbol{U}(t) = \boldsymbol{f}(\boldsymbol{U}_0, t) = \mathrm{e}^{-\boldsymbol{L}t}\boldsymbol{U}_0$ and the *marginal PDF* at time t, $\pi(\boldsymbol{u};t)$, is given by the *causality principle* (lecture #1):

$$\pi_0(\boldsymbol{u}_0) = \pi(\boldsymbol{f}(\boldsymbol{u}_0, t))\det(\boldsymbol{\nabla}_{\boldsymbol{u}}\boldsymbol{f})\,.$$

- It yields the conservation equation of the PDF:

$$0 = \frac{\mathrm{d}\pi_0}{\mathrm{d}t} = \partial_t\pi + \boldsymbol{\nabla}_{\boldsymbol{u}}\cdot(\pi\dot{\boldsymbol{u}}) = \partial_t\pi + \boldsymbol{\nabla}_{\boldsymbol{u}}\cdot\boldsymbol{J}(\pi)$$

with $\boldsymbol{J}$ the probability flux and $\boldsymbol{J}(\pi) = -\pi\boldsymbol{L}\boldsymbol{u}$ the constitutive behavior.

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First-order stochastic differential equation

A general first-order stochastic differential equation for the process $\boldsymbol{U}$ indexed on $\mathbb{R}_+$ with values in $\mathbb{R}^q$:

$$\dot{\boldsymbol{U}}(t) = \boldsymbol{b}(\boldsymbol{U}, t) + \boldsymbol{a}(\boldsymbol{U}, t)\boldsymbol{F}(t)\,, \quad \boldsymbol{U}(0) = \boldsymbol{U}_0\,,$$

with the data:

- $\boldsymbol{u}, t \mapsto \boldsymbol{b}(\boldsymbol{u}, t) : \mathbb{R}^q \times \mathbb{R}_+ \to \mathbb{R}^q$ the *drift* function;
- $\boldsymbol{u}, t \mapsto \boldsymbol{a}(\boldsymbol{u}, t) : \mathbb{R}^q \times \mathbb{R}_+ \to \mathbb{M}_{q,p}(\mathbb{R})$ the *scattering* operator;
- $\boldsymbol{U}_0$ is an r.v. in $\mathbb{R}^q$ with known marginal PDF $\pi_0(\boldsymbol{u}_0)$;
- $\boldsymbol{F}(t) = (F_1(t), \dots F_p(t))$ is a second-order Gaussian random process indexed on $\mathbb{R}$ with values in $\mathbb{R}^p$, also centered, stationary, such that $F_1(t), \dots F_p(t)$ are mutually independent and mean-square continuous, with:

$$\boldsymbol{S}_{\boldsymbol{F}}(\omega) = S_0 \mathbf{1}_{[-B,B]}(\omega)[\boldsymbol{I}_p]\,, \quad S_0 > 0\,, \quad B > 0\,.$$

First-order systems driven by noise

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- $B < +\infty$: colored noise, hot topic!

$$\boldsymbol{U}(t) = \boldsymbol{U}_0 + \int_0^t \boldsymbol{b}(\boldsymbol{U}(s), s)\mathrm{d}s + \int_0^t \boldsymbol{a}(\boldsymbol{U}(s), s)\boldsymbol{F}(s)\mathrm{d}s\,.$$

- $B \to +\infty$: $\boldsymbol{F} \to \dot{\boldsymbol{W}}$ the *normalized Gaussian white noise*, and the solution of the first-oder SDE holds as a "stochastic integral":

$$\boldsymbol{U}(t) = \boldsymbol{U}_0 + \int_0^t \boldsymbol{b}(\boldsymbol{U}(s), s)\mathrm{d}s + \int_0^t \boldsymbol{a}(\boldsymbol{U}(s), s) \circ \mathrm{d}\boldsymbol{W}(s)\,.$$

- *Causality*: the family of r.v. $\{\boldsymbol{U}(s), 0 \leqslant s \leqslant t\}$ is independent of the family of r.v. $\{\boldsymbol{F}(\tau), \tau > t\}$ or $\{\mathrm{d}\boldsymbol{W}(\tau), \tau > t\}$.

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Definition

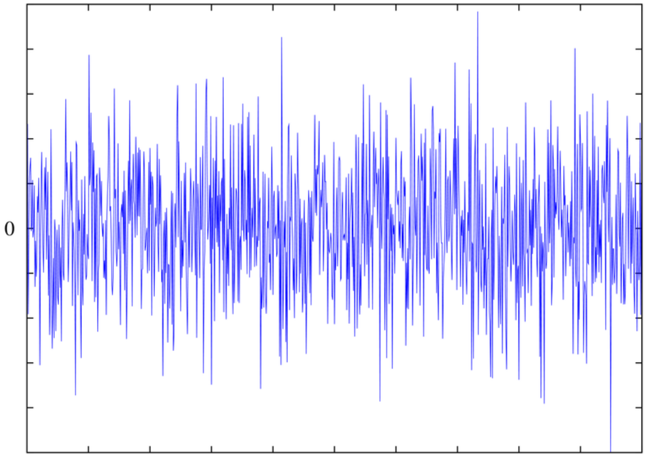
- *The normalized Gaussian white noise* $\boldsymbol{B}(t) \equiv \dot{\boldsymbol{W}}(t)$ *with values in* $\mathbb{R}^p$ *is the Gaussian stochastic process indexed on* $\mathbb{R}$*, centered, stationary, with the spectral density matrix:*

$$\boldsymbol{S}_{\boldsymbol{B}}(\omega) = \frac{1}{2\pi}\boldsymbol{I}_p \,.$$

- *Since* $B_1(t), \dots B_p(t)$ *are uncorrelated and jointly Gaussian, they are mutually independent.*
- $\boldsymbol{B}$ *is not second order* $\|\boldsymbol{B}(t)\|^2 = \int \mathrm{Tr}\, \boldsymbol{S}_{\boldsymbol{B}}(\omega)\mathrm{d}\omega = +\infty$.

This definition holds in the sense of generalized stochastic processes $\varphi \mapsto \boldsymbol{B}(\varphi) : \mathscr{D}(T) \to L^2(\Omega, \mathbb{R}^p)$ where $\mathscr{D}(T)$ is the set of $\mathscr{C}^\infty$ functions having a compact support within $T \subseteq \mathbb{R}$.

White noise
Definition



White noise.

The white noise is the (generalized) derivative of the Wiener process, or *Brownian motion*.

Definition

The (normalized) Wiener process $\boldsymbol{W}(t)$ *with values in* $\mathbb{R}^p$ *is the stochastic process indexed on* $\mathbb{R}_+$*, s.t.:*

- $W_1(t), \dots W_p(t)$ *are mutually independent;*
- $\boldsymbol{W}(0) = \mathbf{0}$ *almost surely (a.s.);*
- *If* $0 \leqslant s < t < +\infty$ *let* $\Delta\boldsymbol{W}(s,t) = \boldsymbol{W}(t) - \boldsymbol{W}(s)$*, then:*
    - $\forall m$ *and* $0 < t_1 < t_2 < \cdots < t_m < +\infty$, $\boldsymbol{W}(0)$, $\Delta\boldsymbol{W}(0,t_1)$, $\Delta\boldsymbol{W}(t_1,t_2)$, ... $\Delta\boldsymbol{W}(t_{m-1},t_m)$ *are mutually independent r.v. (independent increments);*
    - $\Delta\boldsymbol{W}(s,t)$ *is a Gaussian, centered, second-order r.v. with* $\boldsymbol{C}_{\Delta\boldsymbol{W}}(s,t) = (t-s)\boldsymbol{I}_p$.

Wiener process
Characterization

Consequently it can be shown that:

- $\boldsymbol{W}(t)$ is a second-order Gaussian, centered, mean-square continuous, non stationary stochastic process;
- the covariance and conditional PDF for $0 \leqslant t, s < +\infty$:

$$\boldsymbol{C}_{\boldsymbol{W}}(t,s) = \mathrm{Min}(t,s)\boldsymbol{I}_p \,,$$

$$\pi_t(\boldsymbol{v}'; t+s | \boldsymbol{v}; t) = (2\pi s)^{-\frac{p}{2}} \, \mathrm{e}^{-\frac{\|\boldsymbol{v}'-\boldsymbol{v}\|^2}{2s}} \;;$$

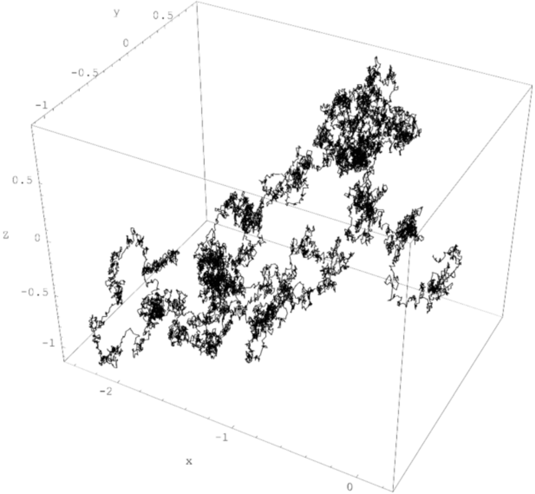
- $\boldsymbol{W}(t)$ has a.s. continuous sample paths;
- sample paths $t \mapsto \boldsymbol{W}(t,\theta)$, $\theta \in \Omega_\theta$, are non differentiable a.s.

As a generalized derivative with $\mathrm{d}\boldsymbol{W} = (\mathrm{d}W_1, \dots \mathrm{d}W_p)$:

$$\mathrm{d}\boldsymbol{W}(\varphi) = \boldsymbol{B}(-\dot{\varphi}) \,, \quad \forall \varphi \in \mathscr{D}(\mathbb{R}) \,.$$

Wiener process

Characterization



Wiener process in $\mathbb{R}^3$.

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- Let $\boldsymbol{X}(t)$ be a stochastic process indexed by $\mathbb{R}_+$ with a.s. continuous sample paths.
- Assume the r.v. $\{\boldsymbol{X}(s), 0 \leqslant s \leqslant t\}$ are independent of the r.v. $\{\Delta \boldsymbol{W}(t,\tau), \tau > t\}$: a *non anticipative* process, then

$$\int_0^t \boldsymbol{X}(s) \mathrm{d}_\lambda \boldsymbol{W}(s)$$

$$= \underset{K\to+\infty}{\mathrm{l.\,i.\,p.}} \sum_{k=1}^{K} \left[(1-\lambda)\boldsymbol{X}(t_k) + \lambda \boldsymbol{X}(t_{k+1})\right] \Delta \boldsymbol{W}(t_k, t_{k+1}) \,,$$

for any partition $0 = t_1 < t_2 < \cdots < t_{K+1} = t$ of $[0,t]$ with $\max_{1\leqslant k\leqslant K}(t_{k+1}-t_k) \underset{K\to+\infty}{\longrightarrow} 0$.

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- A simple example–remind $\Delta W \propto \Delta t^{\frac{1}{2}}$ for the real-valued Wiener process W:

$$\int_0^t W(s)\mathrm{d}_\lambda W(s) = \frac{1}{2}W(t)^2 + \left(\lambda - \frac{1}{2}\right) t\,,$$

from which one deduces the stochastic differential:

$$\mathrm{d}_\lambda(W(t)^2) = 2W(t)\mathrm{d}W(t) + (1-2\lambda)\mathrm{d}t\,.$$

- More generally ($\lambda = 0$ is called the *Itō formula*):

$$\mathrm{d}_\lambda(f(W(t)) = f'(W(t))\mathrm{d}W(t) + \left(\frac{1}{2} - \lambda\right) f''(W(t))\mathrm{d}t\,.$$

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- If $\lambda = \frac{1}{2}$ the usual differential calculus applies, and the solution of SDE holds as a *Stratonovich integral* (1966):

$$\boldsymbol{U}(t) = \boldsymbol{U}_0 + \int_0^t \boldsymbol{b}(\boldsymbol{U}(s), s)\mathrm{d}s + \int_0^t \boldsymbol{a}(\boldsymbol{U}(s), s) \circ \mathrm{d}\boldsymbol{W}(s)\,.$$

- If $\lambda = 0$, its solution holds as an *Itō integral* (1944):

$$\boldsymbol{U}(t) = \boldsymbol{U}_0 + \int_0^t \underline{\boldsymbol{b}}(\boldsymbol{U}(s), s)\mathrm{d}s + \int_0^t \boldsymbol{a}(\boldsymbol{U}(s), s)\mathrm{d}\boldsymbol{W}(s)\,,$$

where:

$$\underline{\boldsymbol{b}}(\boldsymbol{u}, t) = \boldsymbol{b}(\boldsymbol{u}, t) + \frac{1}{2}\boldsymbol{a}^{\mathsf{T}}\boldsymbol{\nabla}_{\boldsymbol{u}}\boldsymbol{a}\,.$$

- $\boldsymbol{U}(t)$ is a *Markov process*.

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- Let $\boldsymbol{U}(t) \in \mathbb{R}^q$ be the solution of the ISDE:

$$\boldsymbol{U}(t) = \boldsymbol{U}_0 + \int_0^t \underline{\boldsymbol{b}}(\boldsymbol{U}(s), s)\mathrm{d}s + \int_0^t \boldsymbol{a}(\boldsymbol{U}(s), s)\mathrm{d}\boldsymbol{W}(s)\,.$$

- Let $\phi : \mathbb{R}^q \times \mathbb{R} \to \mathbb{R}$ be a smooth function. Then *Itō's formula* states that:

$$\begin{aligned}\phi(\boldsymbol{U}(t), t) = \phi(\boldsymbol{U}_0, 0) &+ \int_0^t \frac{\partial \phi}{\partial t}(\boldsymbol{U}(s), s)\mathrm{d}s \\ &+ \int_0^t \boldsymbol{\nabla}_{\boldsymbol{u}}\phi(\boldsymbol{U}(s), s) \cdot \mathrm{d}\boldsymbol{U}(s) \\ &+ \frac{1}{2}\int_0^t \boldsymbol{\nabla}_{\boldsymbol{u}} \otimes \boldsymbol{\nabla}_{\boldsymbol{u}}\phi(\boldsymbol{U}(s), s) : \boldsymbol{a}(\boldsymbol{U}(s), s)\boldsymbol{a}(\boldsymbol{U}(s), s)^{\mathsf{T}}\mathrm{d}s\,,\end{aligned}$$

where $\mathrm{d}\boldsymbol{U}(t) = \underline{\boldsymbol{b}}(\boldsymbol{U}(s), s)\mathrm{d}s + \boldsymbol{a}(\boldsymbol{U}(s), s)\mathrm{d}\boldsymbol{W}(s)$.

Markov processes
Definition

Definition

The conditional probability given $t_0 < \cdots < t_m < t$:

$$\pi_t(\boldsymbol{u};t|\boldsymbol{u}_0,\ldots\boldsymbol{u}_m;t_0,\ldots t_m) = \frac{\pi(\boldsymbol{u}_0,\ldots\boldsymbol{u}_m,\boldsymbol{u};t_0,\ldots t_m,t)}{\pi(\boldsymbol{u}_0,\ldots\boldsymbol{u}_m;t_0,\ldots t_m)}\,.$$

Definition

Let $\boldsymbol{U}(t)$ be a stochastic process defined on $(\Omega,\mathcal{E},P)$ and indexed on $\mathbb{R}_+$ with values in $\mathbb{R}^q$. It is a Markov process if:

- *for all $0 \leqslant t_1 < \cdots < t_m < t$ and $\boldsymbol{u}_1,\ldots\boldsymbol{u}_m,\boldsymbol{u}$ in $\mathbb{R}^q$*

$$\pi_t(\boldsymbol{u};t|\boldsymbol{u}_0,\ldots\boldsymbol{u}_m;t_0,\ldots t_m) = \pi_t(\boldsymbol{u};t|\boldsymbol{u}_m;t_m)\,;$$

- *the marginal PDF $\pi_0(\boldsymbol{u}_0)$ of $\boldsymbol{U}(0)$ can be any PDF.*

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- A Markov process is fully characterized by:
  - its marginal PDF $\pi(\boldsymbol{u};t)$,
  - and its *transition PDF* $\pi_t(\boldsymbol{u};t|\boldsymbol{v};s)$, $0 \leqslant s < t < +\infty$, with

$$\pi(\boldsymbol{u};t) = \int_{\mathbb{R}^q} \pi_t(\boldsymbol{u};t|\boldsymbol{v};s)\pi(\boldsymbol{v};s)\mathrm{d}\boldsymbol{v}\,.$$

- π_t satisfies the *Chapman-Kolmogorov equation*:

$$\pi_t(\boldsymbol{u};t|\boldsymbol{u}';t') = \int_{\mathbb{R}^q} \pi_t(\boldsymbol{u};t|\boldsymbol{v};s)\pi_t(\boldsymbol{v};s|\boldsymbol{u}';t')\mathrm{d}\boldsymbol{v}\,, \quad t' < s < t\,.$$

- Homogeneous Markov process:

$$\pi_t(\boldsymbol{u};t|\boldsymbol{v};s) = \pi_t(\boldsymbol{u};t-s|\boldsymbol{v};0)\,, \quad 0 \leqslant s < t < +\infty\,.$$

- The Brownian motion is a Markov process.

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Definition

The $\mathbb{R}^q$–valued Markov process $\boldsymbol{U}(t)$ with a.s. continuous sample paths and transition PDF $\pi_t(\boldsymbol{v};s|\boldsymbol{u};t)$ is a diffusion process if $\forall\epsilon>0$ (but not necessarily small), $\forall\boldsymbol{u}\in\mathbb{R}^q$ the first moments of its increments are such that for $h>0$:

$$\int_{\|\boldsymbol{v}-\boldsymbol{u}\|\geqslant\epsilon}\pi_t(\mathrm{d}\boldsymbol{v};t+h|\boldsymbol{u};t)=\mathrm{o}(h)\,,$$

$$\int_{\|\boldsymbol{v}-\boldsymbol{u}\|<\epsilon}(\boldsymbol{v}-\boldsymbol{u})\pi_t(\mathrm{d}\boldsymbol{v};t+h|\boldsymbol{u};t)=h\underline{\boldsymbol{b}}(\boldsymbol{u},t)+\mathrm{o}(h)\,,$$

$$\int_{\|\boldsymbol{v}-\boldsymbol{u}\|<\epsilon}(\boldsymbol{v}-\boldsymbol{u})\otimes(\boldsymbol{v}-\boldsymbol{u})\pi_t(\mathrm{d}\boldsymbol{v};t+h|\boldsymbol{u};t)=h\boldsymbol{\sigma}(\boldsymbol{u},t)+\mathrm{o}(h)\,,$$

where $\underline{\boldsymbol{b}}\in\mathbb{R}^q$ and $\boldsymbol{\sigma}\in\mathbb{M}_{q,q}(\mathbb{R})$ symmetric, positive.

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- *Continuity*: particles moving on sample paths of a diffusion process only make small jumps, or the probability of moving a distance ϵ goes to zero as h goes to zero no matter how small ϵ is.
- *Drift*: those particles can have a net mean velocity $\underline{\boldsymbol{b}}$.
- *Diffusion*: particles spread as time increases with the rate $\mathrm{Tr}\,\boldsymbol{\sigma}$. Entropy increases while the phase space contracts, thus some information (energy) gets lost.

$$\boldsymbol{U}(t+h) - \boldsymbol{U}(t) \approx h\underline{\boldsymbol{b}}(\boldsymbol{U}(t),t) + \boldsymbol{\sigma}^{\frac{1}{2}}(\boldsymbol{U}(t),t)\Delta\boldsymbol{W}(t,t+h)\,.$$

Fokker-Planck equation

The marginal PDF π and transition PDF π_t of a diffusion process satisfy the *Fokker-Planck equation*:

$$\partial_t \pi + \boldsymbol{\nabla}_{\boldsymbol{u}} \cdot \left(\pi \underline{\boldsymbol{b}} - \frac{1}{2} \boldsymbol{\nabla}_{\boldsymbol{u}} \cdot (\pi \boldsymbol{\sigma}) \right) = 0 \,,$$

with $\pi(\boldsymbol{u}_0; 0) = \pi_0(\boldsymbol{u}_0)$ and $\lim_{h\downarrow 0} \pi_t(\boldsymbol{u}; t+h|\boldsymbol{v}; t) = \delta(\boldsymbol{u}-\boldsymbol{v})$.

$$\begin{aligned}
\int_{\mathbb{R}^q} f(\boldsymbol{u}) \partial_t \pi_t(\boldsymbol{u}; t|\boldsymbol{v}; s) \mathrm{d}\boldsymbol{u} &= \lim_{h\downarrow 0} \frac{1}{h} \int_{\mathbb{R}^q} f(\boldsymbol{u}) \left(\pi_t(\boldsymbol{u}; t+h|\boldsymbol{v}; s) - \pi_t(\boldsymbol{u}; t|\boldsymbol{v}; s) \right) \mathrm{d}\boldsymbol{u} \\
&= \lim_{h\downarrow 0} \frac{1}{h} \int_{\mathbb{R}^q} \pi_t(\boldsymbol{u}; t|\boldsymbol{v}; s) \left[\int_{\mathbb{R}^q} f(\boldsymbol{u}') \pi_t(\boldsymbol{u}'; t+h|\boldsymbol{u}; t) \mathrm{d}\boldsymbol{u}' - f(\boldsymbol{u}) \right] \mathrm{d}\boldsymbol{u} \qquad \text{(C-K)} \\
&= \lim_{h\downarrow 0} \frac{1}{h} \int_{\mathbb{R}^q} \pi_t(\boldsymbol{u}; t|\boldsymbol{v}; s) \int_{\mathbb{R}^q} \left(f(\boldsymbol{u}') - f(\boldsymbol{u}) \right) \pi_t(\boldsymbol{u}'; t+h|\boldsymbol{u}; t) \mathrm{d}\boldsymbol{u}' \mathrm{d}\boldsymbol{u} \qquad \text{(norm.)} \\
&= \lim_{h\downarrow 0} \frac{1}{h} \int_{\mathbb{R}^q} \pi_t(\boldsymbol{u}; t|\boldsymbol{v}; s) \int_{\|\boldsymbol{u}'-\boldsymbol{u}\|<\epsilon} \left(f(\boldsymbol{u}') - f(\boldsymbol{u}) \right) \pi_t(\boldsymbol{u}'; t+h|\boldsymbol{u}; t) \mathrm{d}\boldsymbol{u}' \mathrm{d}\boldsymbol{u} \,, \quad \forall f \in \mathscr{C}_0^2 \,.
\end{aligned}$$

Then use a Taylor expansion for f, definitions of drift and diffusion, and integrate by parts.

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$$\mathrm{d}\boldsymbol{U} = \underline{\boldsymbol{b}}(\boldsymbol{U},t)\mathrm{d}t + \boldsymbol{a}(\boldsymbol{U},t)\mathrm{d}\boldsymbol{W}\,,\quad \boldsymbol{U}(0) = \boldsymbol{U}_0\,,$$

with the regularity assumptions:

$$\begin{aligned} \|\underline{\boldsymbol{b}}(\boldsymbol{u},t)\| + \|\boldsymbol{a}(\boldsymbol{u},t)\| &\leqslant K(1+\|\boldsymbol{u}\|)\,, \\ \|\underline{\boldsymbol{b}}(\boldsymbol{u}',t) - \underline{\boldsymbol{b}}(\boldsymbol{u},t)\| + \|\boldsymbol{a}(\boldsymbol{u}',t) - \boldsymbol{a}(\boldsymbol{u},t)\| &\leqslant K\|\boldsymbol{u}'-\boldsymbol{u}\|\,. \end{aligned}$$

1. Then the SDE has a unique solution, with a.s. continuous sample paths. If in addition $\underline{\boldsymbol{b}}$ and $\boldsymbol{a}$ are independent of t, $\boldsymbol{U}(t)$ is homogeneous.
2. If $t \mapsto \underline{\boldsymbol{b}}(\boldsymbol{u},t)$ and $t \mapsto \boldsymbol{a}(\boldsymbol{u},t)$ are continuous, $\boldsymbol{U}(t)$ is also a diffusion process with $\boldsymbol{\sigma} = \boldsymbol{a}\boldsymbol{a}^\mathsf{T}$.

Itō's stochastic differential equations (ISDE)

Example: Black-Scholes[1] model

- The relative variation of a stock $U(t)$ with constant (annualized) drift rate μ and volatility σ:

$$\frac{\mathrm{d}U}{U} = \mu \mathrm{d}t + \sigma \mathrm{d}W \,, \quad U(0) = U_0 \,.$$

- Transformation to a Stratonovich SDE:

$$\frac{\mathrm{d}U}{U} = \left(\mu - \frac{\sigma^2}{2}\right) \mathrm{d}t + \sigma \circ \mathrm{d}W \,, \quad U(0) = U_0 \,,$$

for which "normal rules of integration" apply:

$$U(t) = U_0 \, \mathrm{e}^{\sigma W(t) + (\mu - \frac{\sigma^2}{2})t} \,.$$

- The Fokker-Planck equation:

$$\partial_t \pi + \mu \partial_u (\pi u) - \frac{\sigma^2}{2} \partial_u^2 (\pi u^2) = 0 \,, \quad \pi(u; 0) = \pi_0(u) \,.$$

[1] Fischer Black (1938–1995), Myron Scholes (1941–): American financial economists. M. Scholes received the Sveriges Riksbank Prize in Economic Sciences in Memory of A. Nobel in 1997 for this model for valuing options, together with Robert Merton (1944–).

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First-order stochastic differential equation

A general first-order stochastic differential equation for the process $\boldsymbol{U}$ indexed on $\mathbb{R}_+$ with values in $\mathbb{R}^q$:

$$\begin{cases} \dot{\boldsymbol{U}}(t) = \boldsymbol{b}(\boldsymbol{U},t) + \boldsymbol{a}(\boldsymbol{U},t)\boldsymbol{F}(t)\,, & t > 0\,, \\ \boldsymbol{U}(0) = \boldsymbol{U}_0\,, \end{cases}$$

with the data:

- $\boldsymbol{u},t \mapsto \boldsymbol{b}(\boldsymbol{u},t) : \mathbb{R}^q \times \mathbb{R}_+ \to \mathbb{R}^q$ the *drift* function;
- $\boldsymbol{u},t \mapsto \boldsymbol{a}(\boldsymbol{u},t) : \mathbb{R}^q \times \mathbb{R}_+ \to \mathbb{M}_{q,p}(\mathbb{R})$ the *scattering* operator;
- $\boldsymbol{U}_0$ is an r.v. in $\mathbb{R}^q$ with known marginal PDF $\pi_0(\boldsymbol{u}_0)$;
- $\boldsymbol{F}(t) = (F_1(t), \dots F_p(t))$ is a second-order Gaussian random process indexed on $\mathbb{R}^+$ with values in $\mathbb{R}^p$, centered, mean-square continuous.

Markovian realization

Definition

Definition

$\boldsymbol{F}(t)$ *indexed on* $\mathbb{R}^+$ *with values in* $\mathbb{R}^p$, *second-order, Gaussian, centered and mean-square continuous admits a Markovian realization if:*

$$\begin{cases} \boldsymbol{F}(t) = \boldsymbol{H}\boldsymbol{V}(t)\,, & t \geqslant 0\,, \\ \dot{\boldsymbol{V}}(t) = \boldsymbol{P}\boldsymbol{V}(t) + \boldsymbol{Q}\boldsymbol{B}(t)\,, & t > 0\,, \\ \boldsymbol{V}(0) = \boldsymbol{V}_0 & a.s. \end{cases}$$

where $\boldsymbol{V}_0$ *is a Gaussian r.v. in* $\mathbb{R}^n$, $\boldsymbol{V}(t)$ *is a diffusion process indexed on* $\mathbb{R}_+$ *with values in* $\mathbb{R}^n$, $\boldsymbol{P},\boldsymbol{Q} \in \mathbb{M}_n(\mathbb{R})$, $\boldsymbol{H} \in \mathbb{M}_{p,n}(\mathbb{R})$, $\Re\mathrm{e}\{\lambda_j(\boldsymbol{P})\} < 0$.

- This is equivalent to a linear Itō stochastic differential equation.
- $\boldsymbol{V}_0 \sim \mathcal{N}(\boldsymbol{0},\boldsymbol{\Sigma}_0)$ where $\boldsymbol{\Sigma}_0 = \int_0^{+\infty} \mathrm{e}^{\tau\boldsymbol{P}}\boldsymbol{Q}\boldsymbol{Q}^\mathsf{T}\,\mathrm{e}^{\tau\boldsymbol{P}^\mathsf{T}}\,\mathrm{d}\tau$.

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Stochastic Hamiltonians

Definition

$\boldsymbol{F}(t)$ indexed on $\mathbb{R}$ with values in $\mathbb{R}^p$, second-order, mean-square stationary and continuous, centered, is physically realizable if $\exists \mathbb{H} \in L^2(\mathbb{R})$, $\operatorname{supp}\mathbb{H} \subseteq \mathbb{R}_+$, s.t.:

$$\boldsymbol{F}(t) = \int_{-\infty}^{t} \mathbb{H}(t-\tau)\boldsymbol{B}(\tau)\mathrm{d}\tau\,,$$

or equivalently $\boldsymbol{S}_{\boldsymbol{F}}(\omega) = \frac{1}{2\pi}\widehat{\mathbb{H}}(\omega)\widehat{\mathbb{H}}(\omega)^*$, $\forall\omega \in \mathbb{R}$.

A necessary and sufficient condition (Rozanov 1967):

$$\int_{\mathbb{R}} \frac{\ln(\det \boldsymbol{S}_{\boldsymbol{F}}(\omega))}{1+\omega^2}\mathrm{d}\omega > -\infty\,.$$

Markovian realization

Existence for a physically realizable process

Theorem

A necessary and sufficient condition:

$$\boldsymbol{S}_{\boldsymbol{F}}(\omega) = \frac{\boldsymbol{R}(\mathrm{i}\omega)\boldsymbol{R}(\mathrm{i}\omega)^*}{2\pi|P(\mathrm{i}\omega)|^2}\,, \quad \text{or } \mathbb{H}(\omega) = \frac{\boldsymbol{R}(\mathrm{i}\omega)}{P(\mathrm{i}\omega)}\,,$$

where:

- $P(z)$ *is a polynomial of degree* d *on* $\mathbb{C}$ *with real coefficients and roots in the half-plane* $\Re\mathrm{e}(z) < 0$*,*
- $\boldsymbol{R}(z)$ *is a polynomial on* $\mathbb{C}$ *with coefficients in* $\mathbb{M}_{p,n}(\mathbb{R})$ *and degree* $r < n$*.*

The Markovian realization always exists in infinite dimension $n = +\infty$.

First-order SDE (cont'd)

A non linear first-order stochastic differential equation for the process $\boldsymbol{Z}(t) = (\boldsymbol{U}(t), \boldsymbol{V}(t))$ indexed on $\mathbb{R}_+$ with values in $\mathbb{R}^\nu$, $\nu = q + n$:

$$\begin{cases} \mathrm{d}\boldsymbol{Z}(t) = \boldsymbol{b}_z(\boldsymbol{Z}, t)\mathrm{d}t + \boldsymbol{a}_z\mathrm{d}\boldsymbol{W}\,, \quad t > 0\,, \\ \boldsymbol{Z}(0) = \boldsymbol{Z}_0\,, \end{cases}$$

where $\boldsymbol{Z}_0 = (\boldsymbol{U}_0, \boldsymbol{V}_0)$,

$$\boldsymbol{b}_z(\boldsymbol{u}, \boldsymbol{v}, t) = \begin{bmatrix} \boldsymbol{b}(\boldsymbol{u}, t) + \boldsymbol{a}(\boldsymbol{u}, t)\boldsymbol{H}\boldsymbol{v} \\ \boldsymbol{P}\boldsymbol{v} \end{bmatrix}, \quad \boldsymbol{a}_z = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{Q} \end{bmatrix},$$

and $\boldsymbol{W}(t)$ is the Wiener process in $\mathbb{R}^\nu$.

SDE and Fokker-Planck equation

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Introduction

SDE

First-order systems

Stochastic integrals

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Stochastic Hamiltonians

$$\begin{cases} \mathrm{d}U(t) = b(U,t)\mathrm{d}t + a(U,t)\mathrm{d}W(t)\,, & t > 0\,, \\ U(0) = U_0 & \text{a.s.} \end{cases}$$

Definition

An approximation $(\tilde{U}_j)_j$ converges with strong order $k > 0$ if $\exists K_j > 0$:

$$E\left\{\left|U(j\Delta t) - \tilde{U}_j\right|\right\} \leqslant K_j(\Delta t)^k\,.$$

The sample paths of the approximation $\tilde{U}$ should be close to those of the Itō process.

Numerical integration of SDE

Weak convergence

$$\begin{cases} \mathrm{d}U(t) = b(U,t)\mathrm{d}t + a(U,t)\mathrm{d}W(t)\,, & t > 0\,, \\ U(0) = U_0 & \text{a.s.} \end{cases}$$

Definition

An approximation $(\tilde{U}_j)_j$ converges with weak order $k > 0$ if for any polynomial g $\exists K_{g,j} > 0$:

$$\left| E\left\{g(U(j\Delta t))\right\} - E\{g(\tilde{U}_j)\}\right| \leqslant K_{g,j}(\Delta t)^k\,.$$

The probability distribution of the approximation should be close to that of the Itō process in order to get a good estimate of the expectation ($g(u) = u$) or the variance ($g(u) = u^2$), for example.

Time discrete approximations

Explicit 0.5–order methods

- Assume that v and a are independent of time t (thus $U(t)$ is a diffusion process), and let $t_j = j\Delta t$, $b_j = b(\tilde{U}_j)$, $a_j = a(\tilde{U}_j)$, $U_0 \sim \pi_0(\mathrm{d}u_0)$, $G \sim \mathcal{N}(0,1)$.
- Itō SDE: the *Euler-Maruyama scheme* (1955),

$$\begin{aligned}\tilde{U}_{j+1} &= \tilde{U}_j + b_j\Delta t + a_j\sqrt{\Delta t}\,G\,,\\ \tilde{U}_0 &= U_0\,.\end{aligned}$$

- Stratonovich SDE: the *Euler-Heun scheme* (1982),

$$\begin{aligned}\tilde{U}_{j+1} &= \tilde{U}_j + b_j\Delta t + \tilde{a}_j\sqrt{\Delta t}\,G\,,\\ \tilde{a}_j &= \frac{1}{2}\left[a_j + a\left(\tilde{U}_j + a_j\sqrt{\Delta t}\,G\right)\right]\,,\\ \tilde{U}_0 &= U_0\,.\end{aligned}$$

- Both have a strong order $k = \frac{1}{2}$ (vs. $k = 1$ for ordinary differential equations) and a weak order $k = 1$.

Time discrete approximations

Explicit 1–order methods

- The *Milstein scheme* (1974):

$$
\begin{aligned}
\tilde{U}_{j+1} &= \tilde{U}_j + b_{\lambda,j}\Delta t + a_j\sqrt{\Delta t}\,G + \frac{1}{2}a_j a_j'\Delta t(G^2 + 2\lambda - 1)\,, \\
\tilde{U}_0 &= U_0\,,
\end{aligned}
$$

  where $\lambda = 0$ (Itō SDE) or $\lambda = \frac{1}{2}$ (Stratonovich SDE).

- The *Runge-Kutta Milstein scheme* (1984):

$$
\begin{aligned}
\tilde{U}_{j+1} &= \tilde{U}_j + b_{\lambda,j}\Delta t + a_j\sqrt{\Delta t}\,G + \frac{1}{2}a_j \tilde{a}_j'\Delta t(G^2 + 2\lambda - 1)\,, \\
a_j\tilde{a}_j' &= (\Delta t)^{-\frac{1}{2}}\left[a\left(\tilde{U}_j + a_j\sqrt{\Delta t}\right) - a_j\right]\,, \\
\tilde{U}_0 &= U_0\,.
\end{aligned}
$$

- Both have strong and weak orders $k = 1$ (under mild conditions on b and a).

Time discrete approximations

Stochastic Taylor approximations

- Higher-order schemes may be derived using stochastic Taylor expansions:

$$U_{j+1} - U_j = \int_{t_j}^{t_{j+1}} b(U)\mathrm{d}t + \int_{t_j}^{t_{j+1}} a(U)\mathrm{d}W$$

$$\simeq \int_{t_j}^{t_{j+1}} \big(b(U_j) + b'(U_j)\Delta U_j\big)\,\mathrm{d}t + \int_{t_j}^{t_{j+1}} \big(a(U_j) + a'(U_j)\Delta U_j\big)\,\mathrm{d}W\,,$$

where $\Delta U_j = \int_{t_j}^{t} b(U)\mathrm{d}\tau + \int_{t_j}^{t} a(U)\mathrm{d}W$.

- Then $\int_{t_j}^{t_{j+1}}\int_{t_j}^{t} \mathrm{d}_\lambda W(s)\mathrm{d}_\lambda W(t) = \frac{1}{2}(\Delta W)^2 + (\lambda - \frac{1}{2})\Delta t$.
- Higher-order expansions involve additional r.v. $\Delta Z_j = \int_{t_j}^{t_{j+1}}\int_{t_j}^{t} \mathrm{d}W\mathrm{d}t$ with $E\{(\Delta Z_j)^2\} \propto \Delta t^3$ etc.
- Weak Taylor approximations $U_0 \sim \hat{U}_0$, $\Delta W \sim \Delta\hat{W}$, $\Delta Z_j \sim \Delta\hat{Z}_j$ with approximately the same moment properties.

Outline

1 Introduction

2 Stochastic differential equations (SDE)
- First-order stochastic systems driven by noise
- Stochastic integrals
- Diffusion processes

3 Numerical simulations of SDE
- Stochastic modeling with SDE
- Numerical schemes

4 Stochastic Hamiltonian dynamical systems

Canonical equations

- $\boldsymbol{Q} \in \mathbb{R}^q$ the position, $\boldsymbol{P} \in \mathbb{R}^q$ the momentum, $\mathcal{H}$ the Hamiltonian (independent of time), $\boldsymbol{F}$ the non conservative forces,

$$\begin{aligned} \dot{\boldsymbol{Q}} &= \boldsymbol{\nabla}_{\boldsymbol{p}} \mathcal{H}(\boldsymbol{Q}, \boldsymbol{P}) \,, \\ \dot{\boldsymbol{P}} &= -\boldsymbol{\nabla}_{\boldsymbol{q}} \mathcal{H}(\boldsymbol{Q}, \boldsymbol{P}) + \boldsymbol{F}(\boldsymbol{Q}, \boldsymbol{P}, \dot{\boldsymbol{W}}) \,, \end{aligned}$$

  where $\boldsymbol{F}(\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{f}) = -f(\mathcal{H})\mathbf{G}\boldsymbol{\nabla}_{\boldsymbol{p}}\mathcal{H} + g(\mathcal{H})\mathbf{S}\boldsymbol{f}$ and $\dot{\boldsymbol{W}}$ a white noise.

- Example: Duffing oscillator driven by white noise,

$$M\ddot{Q} + D\dot{Q} + KQ + K_0 Q^3 = g_0 S_0 \dot{W}$$

  then $\mathcal{E}_c = \frac{1}{2} M\dot{Q}^2$, $\mathcal{E}_p = \frac{1}{2} KQ^2 + \frac{1}{4} K_0 Q^4$ and $P = \partial_{\dot{q}} \mathcal{E}_c$, thus:

$$\mathcal{H}(Q, P) = \frac{1}{2} M^{-1} P^2 + \frac{1}{2} KQ^2 + \frac{1}{4} K_0 Q^4 \,.$$

Fokker-Planck equation

- The associated *Fokker-Planck equation* for the transition PDF $\pi_t(\boldsymbol{q}', \boldsymbol{p}'; t' | \boldsymbol{q}, \boldsymbol{p}; t)$ reads:

$$\partial_t \pi + \{\pi, \mathcal{H}\} - \boldsymbol{\nabla}_{\boldsymbol{p}} \cdot \boldsymbol{J}(\pi) = 0 \,,$$

with the Poisson bracket and probability flux being defined as:

$$\begin{aligned} \{\pi, \mathcal{H}\} &= \boldsymbol{\nabla}_{\boldsymbol{q}} \pi \cdot \boldsymbol{\nabla}_{\boldsymbol{p}} \mathcal{H} - \boldsymbol{\nabla}_{\boldsymbol{p}} \pi \cdot \boldsymbol{\nabla}_{\boldsymbol{q}} \mathcal{H} \,, \\ \boldsymbol{J}(\pi) &= \pi \left[f(\mathcal{H}) \mathbf{G} + \frac{1}{2} g(\mathcal{H}) g'(\mathcal{H}) \mathbf{S}\mathbf{S}^\mathsf{T} \right] \boldsymbol{\nabla}_{\boldsymbol{p}} \mathcal{H} \\ &\quad + \frac{1}{2} g(\mathcal{H})^2 \mathbf{S}\mathbf{S}^\mathsf{T} \boldsymbol{\nabla}_{\boldsymbol{p}} \pi \,. \end{aligned}$$

Summary

- What's new?
  - Non linear filtering of white noise,
  - A (high-dimensional) PDE for the marginal and transition PDF of diffusion processes,
  - Stochastic integrals,
  - Numerical simulations of SDE,
  - Application to non linear dynamical systems.
- What's left?
  - Numerical solutions of the FKE,
  - Computation of second-order quantities of diffusion processes.

Further reading...

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- D. Talay: Simulation of stochastic differential systems. In *Probabilistic Methods in Applied Physics* (P. Krée & W. Wedig, eds.), pp. 54-96. Lecture Notes in Physics **451**, Springer (1995).