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LECTURE NOTES: INVARIANT DISTRIBUTIONS FOR PARABOLIC SPDES AND THEIR NUMERICAL APPROXIMATIONS

CHARLES-EDOUARD BRÉHIER

Invariant distributions – also referred to as invariant probability distributions – are stationary configurations, in a statistical sense, of stochastic evolution systems (but not in a pathwise sense). In ergodic regimes, they appear as long-time limits, starting from any initial configuration.

To perform numerical simulations, approximations are performed. Natural questions arise, such as: existence and uniqueness of invariant distributions for the discretized systems? speed of convergence to equilibrium? error estimates?

These notes are concerned with these questions for some examples of parabolic, semilinear, Stochastic Partial Differential Equations. Recent work highlights similarities and differences with respect to the finite dimensional situations (SDEs).

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1. Model

Model: parabolic, semilinear, Stochastic Partial Differential Equations

(1)
$$dX(t) = AX(t)dt + F(X(t))dt + \sqrt{2}dW(t) , \quad X(0) = x.$$

We only consider **additive noise** perturbations.

References: some lecture notes [2], [11]. Monograph: [8].

1.1. Setting.

State space. *H* is an infinite dimensional separable Hilbert space.

Notation:

- $|\cdot|$ is the norm, $\langle \cdot, \cdot \rangle$ is the inner product,
- $\|\cdot\|_{\mathcal{L}(H)}$ is the operator norm, on the space of $\mathcal{L}(H)$ of bounded linear operators on H,
- $\|\cdot\|_{\mathcal{L}_2(H)}$ is the Hilbert-Schmidt norm on the space $\mathcal{L}_2(H) \subset \mathcal{L}(H)$ of Hilbert-Schmidt operators on H.

Running example: $H = L^2(0, 1)$.

Linear operator A. There exists a complete orthonormal system $(e_n)_{n\in\mathbb{N}}$ of H - i.e. $\langle e_n, e_m \rangle = \mathbb{1}_{n=m}$ and $\overline{\text{Span} \{e_n, n \in \mathbb{N}\}} = H$ - such that

- $Ae_n = -\lambda_n e_n$, for all $n \in \mathbb{N}$, with $0 < \lambda_1 \le \ldots \le \lambda_n \le \ldots$, $\lambda_n \underset{n \to \infty}{\sim} cn^2 \underset{n \to \infty}{\to} \infty$ for some $c \in (0, \infty)$.

Running example: Ax = x'' for $x \in D(A)$, with domain $D(A) = H^2(0,1) \cap H^1_0(0,1)$ (homogeneous Dirichlet boundary conditions). Then $e_n(\cdot) = \sqrt{2} \sin(\cdot n\pi)$ and $\lambda_n = (\pi n)^2$. Notation: for $\alpha \in [0, 1]$

$$|x|_{\alpha}^{2} := \sum_{n \in \mathbb{N}} \lambda_{n}^{2\alpha} |\langle x, e_{n} \rangle|^{2}, \quad (-A)^{\alpha} x = \sum_{n \in \mathbb{N}} \lambda_{n}^{\alpha} \langle x, e_{n} \rangle e_{n}, \quad \forall x \in D(-A)^{\alpha} = \{z \in H, \ |z|_{\alpha} < \infty\}.$$

Noise: cylindrical Wiener process W. Let a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, with a filtration $(\mathcal{F}_t)_{t>0}$, be fixed.

Define

$$W(t) = \sum_{n \in \mathbb{N}} \beta_n(t) e_n$$

where $(\beta_n)_{n\in\mathbb{N}}$ is a sequence of independent standard one dimensional Wiener processes (adapted to the filtration).

Important remarks:

- the definition does not depend on the choice of the basis of H.
- For any t > 0, $W(t) \notin H$ almost surely.
- If $B \in \mathcal{L}_2(H)$, then the process $(BW(t))_{t>0}$ is well-defined on H.

For $x \in H$, the real-valued process $(\langle W(t), x \rangle)_{t>0}$ is well-defined. It is centered and Gaussian. Correlations:

$$\mathbb{E}\big[\langle W(t), x \rangle \langle W(s), y \rangle\big] = \min(t, s) \langle x, y \rangle.$$

Noise is white in space: $\langle W(t), x \rangle$ and $\langle W(t), y \rangle$ are independent if $\langle x, y \rangle = 0$, in particular if x and y have disjoint supports. Other interpretation: Fourier components $\langle W(t), e_n \rangle = \beta_n(t)$ are statistically identical.

Let us discuss interpretation in terms of Space-time white noise: note that W(t) = $\langle \xi, \mathbb{1}_{[0,t]} \rangle_{L^2(\mathbb{R}^+)}$ is formally the antiderivative in time of the space-time white noise

$$\xi = \sum_{k,n \in \mathbb{N}} \gamma_{k,n} f_k \otimes e_n$$

where $(f_k)_{k\in\mathbb{N}}$ is a complete orthonormal system of $L^2(\mathbb{R}^+)$, and $(\gamma_{n,k})_{k,n\in\mathbb{N}}$ are independent standard Gaussian random variables. Correlations: formally $\mathbb{E}[\xi(t,\theta)\xi(s,\eta)] = \delta_{ts}\delta_{\theta\eta}$.

In this notes, we only consider cylindrical Wiener process – space-time white noise. This results in processes with low regularity properties. One way to increase regularity would be to add spatial correlations (with a Q-Wiener processes instead). Some of the results extend easily, some do not remain true – let us mention the expression of the invariant distribution for gradient type SPDEs.

Nonlinear coefficient F. The function $F: H \to H$ is assumed globally Lipschitz continuous, and bounded.

For the analysis of the error in numerical schemes, more regularity will be required.

Running example: $F(x)(\cdot) = f(x(\cdot))$ on (0,1), with $f : \mathbb{R} \to \mathbb{R}$ bounded and globally Lipschitz continuous.

1.2. Mild solutions, global well-posedness.

Linear equation, semi-group. Solving the linear PDE $\dot{x} = Ax$ with initial condition x_0 :

$$x(t) = e^{tA}x_0 = \sum_{n \in \mathbb{N}} e^{-t\lambda_n} \langle x_0, e_n \rangle e_n.$$

True not only for $x_0 \in D(A)$, but also for $x_0 \in H$.

Parabolic effects:

• Regularization: for $\alpha \in [0, 1]$, and $t \in (0, \infty)$,

$$\|(-A)^{\alpha}e^{tA}\|_{\mathcal{L}(H)} \le \frac{c_{\alpha}}{(t\wedge 1)^{\alpha}},$$

with $c_{\alpha} \in (0, \infty)$.

• Dissipation:

$$\|e^{tA}\|_{\mathcal{L}(H)} \le e^{-\lambda_1 t}.$$

Long-time behaviour: for any initial condition $x_0 \in H$, exponentially fast,

$$e^{tA}x_0 \xrightarrow[t \to \infty]{} 0.$$

Stochastic convolution. Meaning of solving the SPDE $dX = AXdt + \sqrt{2}dW(t)$?

Mild solution (with initial condition 0):

$$W_A(t) = \int_0^t e^{(t-s)A} \sqrt{2} dW(s),$$

called the stochastic convolution.

In components: independent Ornstein-Uhlenbeck processes,

$$\langle W_A(t), e_n \rangle = \int_0^t e^{-\lambda_n(t-s)} \sqrt{2} d\beta_n(s),$$

solutions of $dx_n = -\lambda_n x_n dt + \sqrt{2} d\beta_n(t)$.

Why is this well-defined: (infinite dimensional version of Itô's isometry formula)

$$\mathbb{E}|W_A(t)|^2 = 2\int_0^t \|e^{(t-s)A}\|_{\mathcal{L}_2(H)}^2 ds = 2\sum_{n\in\mathbb{N}}\int_0^t |e^{(t-s)A}e_n|^2 ds = \sum_{n\in\mathbb{N}}\frac{1}{\lambda_n} \left(1 - e^{-2\lambda_n t}\right) < \infty.$$

Regularity properties:

- sup $\mathbb{E}|W_A(t)|^2_{\alpha} < \infty$ if and only if $\alpha \in [0, \frac{1}{4})$.
- $\mathbb{E}|W_A(t) W_A(s)|^2 \leq C_{\kappa}|t-s|^{\frac{1}{2}-\kappa}$, for all $\kappa \in (0, \frac{1}{2})$. In the *running example*: trajectories of W_A are $\frac{1}{4} \kappa$ Hölder continuous in time, $\frac{1}{2} - 2\kappa$ Hölder continuous in space. Notice the parabolic scaling.

Note the useful inequality (which may be combined with the regularization estimate above):

$$|e^{tA} - e^{sA}||_{\mathcal{L}(H)} \le C_{\alpha}|t-s|^{\alpha}||e^{\min(t,s)A}||_{\mathcal{L}(H,D((-A)^{\alpha}))}.$$

Mild solutions for the semilinear SPDE. Let $x_0 \in H$. There exists a unique adapted process $(X(t))_{t>0}$, continuous, with values in H, which satisfies, for all $t \ge 0$,

$$X(t) = e^{tA}x_0 + \int_0^t e^{(t-s)A}F(X(s))ds + \sqrt{2}\int_0^t e^{(t-s)A}dW(s).$$

This process is the unique mild solution of the semilinear SPDE

$$dX = AXdt + F(X)dt + \sqrt{2}dW(t) , \quad X(0) = x_0.$$

Since noise is additive, $X(t) = R(t) + W_A(t)$, where $(R(t))_{t \ge 0}$ solves the random PDE

$$\frac{dR(t)}{dt} = AR(t) + F(R(t) + W_A(t)) , \quad R(0) = x_0.$$

Same regularity properties as the stochastic convolution (for positive times, if the initial condition x_0 is not sufficiently regular).

Example of estimate: for $\alpha \in [0, \frac{1}{4})$, and $T \ge 0$, for all $t \in (0, T]$,

$$\mathbb{E}|(-A)^{\alpha}X(t)|^{2} \leq C_{\alpha}(T)\left(1 + \frac{|x_{0}|^{2}}{t^{2\alpha}}\right).$$

2. Invariant distributions: existence, uniqueness, convergence

Assume that the initial condition of the SPDE is random (and independent of the noise $(W(t))_{t>0}$). For positive times t, what is the law of X(t)? What happens when $t \to \infty$?

References (not exhaustive, but sufficient for our purpose; see references therein): [9],[7].

2.1. **Definition.** The solution of the SPDE is a Markov process. Introduce the evolution semigroup $(P_t)_{t>0}$, by

$$P_t\varphi(x) = \mathbb{E}_x\big[\varphi(X(t))\big]$$

for bounded measurable functions $\varphi : H \to \mathbb{R}$, where \mathbb{E}_x denotes the expectation, assuming the initial condition is X(0) = x. The Markov property means that $P_{t+s} = P_t P_s$ for all $t, s \ge 0$.

If X(0) has distribution μ_0 , then X(t) has distribution μ_t given by the equivalent formulations

$$\int \varphi d\mu_t = \int P_t \varphi d\mu_0 , \quad \mu_t = P_t^* \mu_0$$

A distribution μ is invariant if

$$\mu_0 = \mu \implies \mu_t = \mu, \quad \forall \ t \ge 0.$$

Questions: existence, uniqueness? convergence to invariant distributions starting from an arbitrary distribution?

Some particular cases:

- Assume F = 0. Then the SPDE $dX = AXdt + \sqrt{2}dW(t)$ admits a (unique, as explained below) invariant distribution ν_{∞} , which is Gaussian, centered, and has co-variance operator $(-A)^{-1}$. More explicitly, ν_{∞} is the law of the *H*-valued random variable $\sum_{n \in \mathbb{N}} \frac{\gamma_n}{\sqrt{\lambda_n}} e_n$ where $(\gamma_n)_{n \in \mathbb{N}}$ are independent standard Gaussian random variables. Verification is straightforward.
- Assume F = -DV is the Fréchet derivative of a \mathcal{C}^1 function $V : H \to \mathbb{R}$. Then the SPDE $dX = AXdt DV(X)dt + \sqrt{2}dW(t)$ admits a (unique) invariant distribution

$$\mu_{\infty}(dx) = Z^{-1}e^{-V(x)}\nu_{\infty}(dx),$$

when the normalizing constant $Z = \int_H e^{-V(y)} \nu_{\infty}(dy)$ is well-defined, in $(0, \infty)$ – for instance, if V is bounded.

Note that this formula is valid only when considering space-time white noise perturbation.

Running example: ν_{∞} is the law of a Brownian Bridge on (0,1), μ_{∞} is the law of a conditioned diffusion.

2.2. Existence. The general strategy is based on the Krylov-Bogoliubov criterion. For precise statements, see for instance [9, Section 3.1], [7, Theorem 5, Chapter 2].

The ideas are as follows. Let $x_0 \in H$ be an arbitrary initial condition. Since F is assumed to be bounded, one shows the uniform in time moment estimate below: for all $t \ge 0$,

$$\mathbb{E}|(-A)^{\alpha}X(t)|^{2} \le C_{\alpha}\left(1 + \frac{|x_{0}|^{2}}{t^{2\alpha}}\right)$$

with $C_{\alpha} \in (0, \infty)$ for all $\alpha \in (0, \frac{1}{4})$.

Moreover, note that for every $R \in (0, \infty)$, the set

$$\left\{ x \in H; \ \sum_{n=1}^{\infty} \lambda_n^{2\alpha} |\langle x, e_n \rangle|^2 \le R \right\}$$

is compact (in *H*, for the $|\cdot|$ norm) when $\alpha \in (0, \frac{1}{4})$ – but, of course, not when $\alpha = 0$.

As a consequence, the family of distributions $(\pi_t)_{t>0}$ defined by

$$\pi_t = \frac{1}{t} \int_0^t P_s^\star \delta_{x_0} ds$$

is tight. By Prokhorov's Theorem, let

$$\pi = \lim_{n \to \infty} \pi_{t_n}$$

for some increasing sequence $t_n \to \infty$. In other words, for all bounded and continuous $\varphi: H \to \mathbb{R}, \int \varphi d\pi_{t_n} \xrightarrow[n \to \infty]{} \int \varphi d\pi$.

It remains to prove that π is an invariant distribution. Another assumption is required: the semigroup $(P_t)_{t\geq 0}$ is Feller. This means that, for any $t\geq 0$, if $\varphi: H \to \mathbb{R}$ is continuous and bounded, then $P_t\varphi$ is continuous (and bounded). In our case, the semigroup is indeed Feller. Let t > 0. On the one hand, $P_t^* \pi_{t_n} \xrightarrow[n \to \infty]{} P_t^* \pi$. Observe that the Feller property is crucial to get this convergence. On the other hand,

$$P_t^{\star} \pi_{t_n} = \frac{1}{t_n} \int_t^{t+t_n} P_s^{\star} \delta_{x_0} ds$$
$$= \pi_{t_n} + \frac{1}{t_n} \left(\int_{t_n}^{t+t_n} P_s^{\star} \delta_{x_0} ds - \int_0^t P_s^{\star} \delta_{x_0} ds \right)$$
$$\xrightarrow[n \to \infty]{} \pi.$$

Thus $P_t^{\star}\pi = \pi$, for all $t \ge 0$, which concludes the proof that π is an invariant distribution.

The arguments given above can also be applied for the discretized systems considered in the sequel.

2.3. Uniqueness. A general criterion is Doob's Theorem: strong Feller property and irreducibility imply the uniqueness of the invariant distribution. In our context, this strategy applies because the noise is non-degenerate: it is a cylindrical Wiener process.

When noise is degenerate (for instance even when a finite number of modes are forced), the situation is much more difficult than for SDEs: see the works of Hairer-Mattingly (asymptotic strong Feller property, hypoellipticity in infinite dimension), Kuksin-Shirikyan...

When considering a discrete space version, results for SDEs apply. On the contrary, up to my knowledge, the application of these arguments in the discrete-time setting, in the infinite dimensional framework, has not been performed so far, and is an open question.

Under a stronger assumption given below, much simpler arguments yield the uniqueness property. In addition, their application to the time-discretized systems is straightforward. In the sequel, we will thus assume that

$$\operatorname{Lip}(F) = \mathcal{L}_F < \lambda_1.$$

Consider two arbitrary initial conditions $x_1, x_2 \in H$, and a single realization of the driving noise process $(W(t))_{t\geq 0}$. Let $(X(t, x_1))_{t\geq 0}$ and $(X(t, x_2))_{t\geq 0}$ denote the solutions of the SPDE, with $X(0, x_1) = x_1$ and $X(0, x_2) = x_2$. Then, almost surely,

$$\frac{1}{2}\frac{d|X(t,x_2) - X(t,x_1)|^2}{dt} \le -(\lambda_1 - \mathcal{L}_F)|X(t,x_2) - X(t,x_1)|^2,$$

and, thanks to Gronwall's lemma, for all $t \ge 0$

$$\mathbb{E}|X(t,x_2) - X(t,x_1)|^2 \le e^{-2(\lambda_1 - \mathcal{L}_F)t} |x_2 - x_1|^2.$$

Uniqueness of the invariant distribution is then straightforward.

2.4. Convergence. Consider an arbitrary initial condition $x_0 \in H$, and assume $L_F < \lambda_1$. Let $\varphi : H \to \mathbb{R}$ be Lipschitz continuous. Then

$$\left|\mathbb{E}\left[\varphi(X(t,x_0))\right] - \int \varphi d\mu_{\infty}\right| \le C(\varphi,|x_0|)e^{-(\lambda_1 - \mathcal{L}_F)t},$$

in other words, convergence to equilibrium is exponentially fast. In addition, the unique invariant distribution μ_{∞} is ergodic.

For our purpose of estimating $\int \varphi d\mu_{\infty}$, this can be interpreted as follows: $\varphi(X(t, x_0))$ is an estimator of that quantity, with a bias which vanishes exponentially fast when t is large. For a given error, this gives a way of choosing t.

This is a nice and important property, which we would like to be preserved by discretization schemes.

3. Numerical schemes

A recent monograph: [13], see also references therein.

Goal: simulatable schemes to estimate averages $\mu_{\infty}(\varphi) = \int_{H} \varphi d\mu_{\infty}$, and provide error bounds, for (large?) classes of test functions φ .

Several discretizations are necessary:

- space discretization of
 - the solution: values in a finite dimensional space
 - the noise: truncate the series,
- time discretization of
 - the solution: build a discrete-time Markov chain
 - the noise: use increments.

Fully or semi-discrete approximations may be considered, and may be studied in the same framework.

Let us introduce discretization parameters: space dimension $N \in \mathbb{N}$, time step size $\Delta t \in$ (0, 1).

3.1. Definitions.

Space-discretization. In these notes, we consider the spectral Galerkin method only. For $N \in \mathbb{N}$. let

$$H_N = \operatorname{span} \{e_1, \ldots, e_N\},\$$

and $P_N \in \mathcal{L}(H)$ the associated orthogonal projection. Note that $||P_N||_{\mathcal{L}(H)} = 1$.

Discretization of the noise consists in replacing the infinite sum $W(t) = \sum_{n \in \mathbb{N}} \beta_n(t) e_n$ with the finite sum $\sum_{n=1}^{N} \beta_n(t) e_n = P_N W(t)$. Discretization of the equation consists in replacing F with $P_N F$, and dW with $P_N dW$.

Spectral Galerkin scheme:

$$dX^{N}(t) = AX^{N}(t)dt + P_{N}F(X^{N}(t))dt + \sqrt{2}P_{N}dW(t) , \quad X^{N}(0) = P_{N}X(0).$$

Mild formulation:

$$X^{N}(t) = e^{tA} P_{N} X(0) + \int_{0}^{t} e^{(t-s)A} P_{N} F(X^{N}(s)) ds + \sqrt{2} P_{N} \int_{0}^{t} e^{(t-s)A} dW(s).$$

Since H_N is a finite dimensional space, with dimension N, X^N may be considered as the solution of a SDE.

In practice, general Finite Element methods are more useful than the spectral Galerkin method: anyway, this is a good toy model, which is important for the analysis of all schemes. The analysis is simpler, since projection operators P_N commute with A and e^{tA} .

Time-discretization. Let $\Delta t \in (0, 1)$ (the assumption $\Delta t < 1$ is only for convenience).

We consider discretization by the linear implicit Euler scheme.

First, increments of the noise are denoted by

$$\Delta W_n = W((n+1)\Delta t) - W(n\Delta t).$$

The scheme is then defined by

$$X_{n+1}^{\Delta t} = X_n^{\Delta t} + \Delta t A X_{n+1}^{\Delta t} + \Delta t F(X_n^{\Delta t}) + \sqrt{2} \Delta W_n$$
$$= S_{\Delta t} X_n^{\Delta t} + \Delta t S_{\Delta t} F(X_n^{\Delta t}) + \sqrt{2} S_{\Delta t} \Delta W_n,$$

where $S_{\Delta t} = (I - \Delta t A)^{-1}$. Only the second line makes sense. Initial condition is $X_0^{\Delta t} = x_0$. This scheme is well-defined, indeed $S_{\Delta t}$ is an Hilbert-Schmidt operator: $\Delta W_n \notin H$, but

 $\mathbb{E}|S_{\Delta t}\Delta W_n|^2 = \Delta t ||S_{\Delta t}||^2_{\mathcal{L}_2(H)}$, with

$$||S_{\Delta t}||^2_{\mathcal{L}_2(H)} = \sum_{n=1}^{\infty} \frac{1}{(1+\lambda_n \Delta t)^2} < \infty.$$

Moreover, $S_{\Delta t}$ is a "nice approximation" of $e^{\Delta tA}$. For instance, note that $\|S_{\Delta t}\|_{\mathcal{L}(H)} = \frac{1}{1+\lambda_1\Delta t}$.

There is a version of the mild formulation, which is useful to prove moment bounds (and ultimately error estimates):

$$X_{n}^{\Delta t} = S_{\Delta t}^{n} + \Delta t \sum_{k=0}^{n-1} S_{\Delta t}^{n-k} F(X_{k}^{\Delta t}) + \sqrt{2} \sum_{k=0}^{n-1} S_{\Delta t}^{n-k} \Delta W_{k}.$$

Note that an explicit discretization is not appropriate, for (at least) two reasons: the noise W(t) does not take values in H, and the explicit discretization of $\dot{x} = Ax$ does not make sense.

Full-discretization. Combining space and time discretization schemes is possible: the full-discretization scheme is defined by

$$X_{n+1}^{N,\Delta t} = S_{\Delta t} X_n^{N,\Delta t} + \Delta t S_{\Delta t} P_N F(X_n^{N,\Delta t}) + \sqrt{2} S_{\Delta t} P_N \Delta W_n.$$

Note that P_N commutes with $S_{\Delta t}$, which simplifies the definition and the analysis of the scheme.

The discretization parameters N and Δt are independent of each other. In the sequel, we consider the discretization separately, however it is straightforward to adapt the approach and the results for the full-discretization scheme.

3.2. Invariant distributions.

Existence. It is sufficient to assume that F is bounded. Proof follows the Krylov-Bogoliubov strategy, thanks to appropriate moment bounds.

• Space-discretization. Note that X^N takes values in the finite dimensional space H_N : proving that for fixed N

$$\sup_{t\geq 0} \mathbb{E}|X^N(t)|^2 < \infty$$

is sufficient to obtain the required tightness (all norms are equivalent, thus no need of $\alpha > 0$).

• <u>Time-discretization</u>. The state space is the infinite dimensional space H, thus it is necessary to consider $\mathbb{E}|(-A)^{\alpha}X_n^{\Delta t}|^2$, with $\alpha > 0$. Observe that $X_n^{\Delta t} = R_n^{\Delta t} + Z_n^{\Delta t}$, where $(Z_n^{\Delta t})_{n\geq 0}$ is the solution of the equation when F = 0 (and thus approximates the stochastic convolution)

$$Z_{n+1}^{\Delta t} = S_{\Delta t} Z_n^{\Delta t} + \sqrt{2} S_{\Delta t} \Delta W_n , \quad , Z_0^{\Delta t} = 0,$$

and

$$R_{n+1}^{\Delta t} = S_{\Delta t} R_n^{\Delta t} + \Delta t S_{\Delta t} F(R_n^{\Delta t} + Z_n^{\Delta t}).$$

On the one hand,

$$\mathbb{E}|(-A)^{\alpha}Z_{n}^{\Delta t}|^{2} = 2\Delta t \sum_{k=0}^{n-1} ||(-A)^{\alpha}S_{\Delta t}^{n-k}||_{\mathcal{L}_{2}(H)}^{2}$$
$$\leq \sum_{p=1}^{\infty} \frac{2\lambda_{p}^{2\alpha}}{\lambda_{p}(2+\lambda_{p}\Delta t)} \left(1 - \frac{1}{(1+\lambda_{p}\Delta t)^{2n}}\right)$$

thus, for all $\alpha \in [0, \frac{1}{2})$

$$\sup_{n\geq 0} \mathbb{E}|(-A)^{\alpha} Z_n^{\Delta t}|^2 \leq M_{\alpha,\Delta t} < \infty.$$

Observe that $\alpha \in [\frac{1}{4}, \frac{1}{2})$ is allowed: however, uniform results with respect to the time step size $\Delta t \in (0, 1)$ only hold true when $\alpha < \frac{1}{4}$, consistently with the continuous-time limit:

$$\sup_{\Delta t \in (0,1)} M_{\alpha,\Delta t} < \infty \iff \alpha \in [0, \frac{1}{4}).$$

On the other hand,

$$\mathbb{E}|(-A)^{\alpha}R_{n}^{\Delta t}|^{2} \leq 2|(-A)^{\alpha}S_{\Delta t}^{n}x_{0}|^{2} + 2\Delta t\sum_{k=0}^{n-1}\mathbb{E}|(-A)^{\alpha}S_{\Delta t}^{n-k}F(X_{k}^{\Delta t})|^{2}$$
$$\leq \frac{C_{\alpha}|x_{0}|^{2}}{(n\Delta t)^{2\alpha}} + C\Delta t\sum_{k=0}^{n-1}\|(-A)^{\alpha}S_{\Delta t}^{n-k}\|_{\mathcal{L}(H)}^{2}$$
$$\leq C_{\alpha}\left(1 + \frac{|x_{0}|^{2}}{(n\Delta t)^{2\alpha}}\right).$$

Combining the estimates, for $\alpha \in (0, \frac{1}{4})$, there exists $C_{\alpha} \in (0, \infty)$, such that for all $n \in \mathbb{N}$

$$\mathbb{E}|(-A)^{\alpha}X_n^{\Delta t}|^2 \le C_{\alpha}\left(1 + \frac{|x_0|^2}{(n\Delta t)^{2\alpha}}\right),$$

and the Krylov-Bogoliubov criterion may then be applied.

Uniqueness. First, what can be said with only the assumption that F is bounded?

• Space discretization. For $N \in \mathbb{N}$, the stochastic evolution equation is a SDE, with values in the finite dimensional space N. The diffusion is non-degenerate, the Doob's criterion thus applies. The generator \mathcal{L}^N of the diffusion is an elliptic operator, one may directly look at the equation $(\mathcal{L}^N)^* \rho_N = 0$, which admits a unique solution such that $\int \rho_N(x) dx = 1$.

• <u>Full discretization</u>. For fixed $N \in \mathbb{N}$, the process $(X_n^{N,\Delta t})_{n\geq 0}$ can be shown to have a unique invariant distribution, for sufficiently small Δt , precisely for $\Delta t \in (0, \Delta t_N)$. This comes from application of SDE results, see for instance [14].

However, up to my knowledge, it is an open question to determine whether

$$\inf_{N\in\mathbb{N}} \Delta t_N > 0 \quad \text{or} \quad \inf_{N\in\mathbb{N}} \Delta t_N = 0.$$

• Time discretization. It corresponds to taking the limit $N \to \infty$ in the full discretization scheme. The answer is not known, it depends on the solution to the above question above.

Let us now add the assumption $L_F < \lambda_1$. Uniqueness and exponential convergence are then obtained by straightforward arguments.

• Space discretization. Thanks to the equality $||P_N||_{\mathcal{L}(H)} = 1$, one obtains again

$$|X^{N}(t, x_{2}) - X^{N}(t, x_{1})| \le e^{-(\lambda_{1} - \mathbf{L}_{F})t} |x_{2} - x_{1}|,$$

with solutions driven by the same noise process. Uniqueness and exponential convergence follows.

• Time discretization. One obtains

$$|X_n^{\Delta t}(x_2) - X_n^{\Delta t}(x_1)| \le \frac{(1 + \mathcal{L}_F \Delta t)^n}{(1 + \lambda_1 \Delta t)^n} |x_2 - x_1| \le e^{-\frac{(\lambda_1 - \mathcal{L}_F)}{1 + \lambda_1 \Delta t} n\Delta t} |x_2 - x_1|,$$

for solutions driven by the same noise process, starting from different initial conditions $x_1, x_2 \in H$. Uniqueness and exponential convergence follows.

• Full discretization. Straightforward by combining the two cases.

Conclusion. For $N \in \mathbb{N}$ and $\Delta t \in (0, 1)$, there exists unique invariant distributions

- μ^N_∞, space discretization,
 μ^{Δt}_∞, time discretization,
 μ^{N,Δt}_∞, full discretization.

Moreover, for Lipschitz continuous functions $\varphi: H \to \mathbb{R}$, and all $t \ge 0$ and $n \ge 0$,

$$\left|\mathbb{E}\varphi(X^{N}(t)) - \int \varphi d\mu_{\infty}^{N}\right| \leq C(\varphi, |x_{0}|)e^{-(\lambda_{1}-\mathbf{L}_{F})t},$$
$$\left|\mathbb{E}\varphi(X_{n}^{\Delta t}) - \int \varphi d\mu_{\infty}^{\Delta t}\right| \leq C(\varphi, |x_{0}|)e^{-\frac{(\lambda_{1}-\mathbf{L}_{F})}{1+\lambda_{1}\Delta t}n\Delta t}.$$

4. Analysis of the error

It remains to study the discretization error (bias)

$$\int \varphi d\mu_{\infty}^{N} - \int \varphi d\mu_{\infty} \quad , \quad \int \varphi d\mu_{\infty}^{\Delta t} - \int \varphi d\mu_{\infty},$$

for classes of functions $\varphi: H \to \mathbb{R}$ to be identified.

A first step is to study the case F = 0: the invariant distributions are Gaussian, explicit computations can be performed and identification of the orders of convergence is easily done.

The second step is to generalize these results in the semilinear case, $F \neq 0$. The analysis is much more complicated, but the situation is rather well-understood now.

4.1. The Gaussian case. Assume F = 0, *i.e.* consider the SPDE

$$dZ(t) = AZ(t)dt + \sqrt{2}dW(t).$$

Invariant distributions of the numerical approximations: let $N \in \mathbb{N}$, $\Delta t \in (0, 1)$,

- $\nu_{\infty} = \mu_{\infty}$ is the centered Gaussian distribution on H, with covariance operator $Q_{\infty} =$ $(-A)^{-1}$
- $\nu_{\infty}^{N} = \mu_{\infty}^{N}$ is the centered Gaussian distribution on H, with covariance operator $Q_{\infty}^{N} =$
- $P_{N}^{\infty}(-A)^{-1}P_{N},$ $\nu_{\infty}^{\Delta t} = \mu_{\infty}^{\Delta t}$ is the centered Gaussian distribution on H, with covariance operator $Q_{\infty}^{\Delta t} = (-A)^{-1} \left(I \frac{\Delta t}{2}A\right)^{-1}.$

More explicitly: let $(\gamma_p)_{p \in \mathbb{N}}$ denote independent standard real-valued Gaussian random variables. Then

• ν_{∞} is the law of $\sum_{p \in \mathbb{N}} \frac{1}{\sqrt{\lambda_p}} \gamma_p e_p$,

Regularity of test functions $\varphi : H \to \mathbb{R}$ matters: the order of convergence depends on control of derivatives. Notation:

$$\begin{aligned} \|\varphi\|_0 &= \sup_{x \in H} |\varphi(x)|, \\ \|\varphi\|_1 &= \|\varphi\|_0 + \sup_{x \neq y \in H} \frac{|\varphi(x) - \varphi(y)|}{|x - y|}, \\ \|\varphi\|_2 &= \sup_{x \in H} |\varphi(x)| + \sup_{x \in H} |D\varphi(x)|_H + \sup_{x \in H} \|D^2\varphi(x)\|_{\mathcal{L}(H)}. \end{aligned}$$

Theorem 1. For any $\kappa \in (0, \frac{1}{2})$, there exists $C_{\kappa} \in (0, \infty)$ such that for all functions φ : $H \to \mathbb{R}$ of class \mathcal{C}^2 ,

$$\left|\int \varphi d\nu_{\infty}^{N} - \int \varphi d\nu_{\infty}\right| \leq C_{\kappa} \|\varphi\|_{2} \frac{1}{\lambda_{N}^{\frac{1}{2}-\kappa}} \quad , \quad \left|\int \varphi d\nu_{\infty}^{\Delta t} - \int \varphi d\nu_{\infty}\right| \leq C_{\kappa} \|\varphi\|_{2} \Delta t^{\frac{1}{2}-\kappa}.$$

The proof of this result is straightforward (but is specific to the Gaussian case). It follows the arguments from [5, Lemma 3.4]. As mentioned during the lectures, by Dr. Zhihui Liu, in that result one may in fact choose $\kappa = 0$.

The order of convergence $\frac{1}{2}$ is optimal: use the test function $\varphi(x) = \exp(-|x|^2)$, see [5, Remark 3.1]. precisely, one way of writing this result is as follows:

$$\begin{split} &\limsup_{N \to \infty} \, \lambda_N^r \sup_{\|\phi\|_2 \le 1} |\int \phi d\nu_\infty - \int \phi d\nu_\infty^N| = \begin{cases} 0, \ \forall \ r \in [0, \frac{1}{2}) \\ \infty, \ \forall \ r \in (\frac{1}{2}, 1) \end{cases} , \\ &\limsup_{\Delta t \to 0} \, \frac{1}{\Delta t^r} \sup_{\|\phi\|_2 \le 1} |\int \phi d\nu_\infty - \int \phi d\nu_\infty^{\Delta t}| = \begin{cases} 0, \ \forall \ r \in [0, \frac{1}{2}) \\ \infty, \ \forall \ r \in (\frac{1}{2}, 1) \end{cases} , \end{split}$$

For less regular test functions, orders of convergence need to be modified. See [3].

Theorem 2. If bounded continuous test functions $\varphi : H \to \mathbb{R}$ are considered, there is no order of convergence:

$$\limsup_{N \to \infty} \sup_{\|\phi\|_0 \le 1} |\int \phi d\nu_{\infty} - \int \phi d\nu_{\infty}^N| > 0 \quad , \quad \limsup_{\Delta t \to 0} \sup_{\|\phi\|_0 \le 1} |\int \phi d\nu_{\infty} - \int \phi d\nu_{\infty}^{\Delta t}| > 0.$$

If bounded Lipschitz continuous test functions are considered, the order of convergence is $\frac{1}{4}$:

$$\begin{split} \limsup_{N \to \infty} \lambda_N^r \sup_{\|\phi\|_1 \le 1} |\int \phi d\nu_\infty - \int \phi d\nu_\infty^N| &= \begin{cases} 0, \ \forall \ r \in [0, \frac{1}{4}) \\ \infty, \ \forall \ r \in (\frac{1}{4}, \frac{1}{2}) \end{cases} \\ \\ \limsup_{\Delta t \to 0} \frac{1}{\Delta t^r} \sup_{\|\phi\|_1 \le 1} |\int \phi d\nu_\infty - \int \phi d\nu_\infty^{\Delta t}| &= \begin{cases} 0, \ \forall \ r \in [0, \frac{1}{4}) \\ \infty, \ \forall \ r \in (\frac{1}{4}, \frac{1}{2}) \end{cases} \end{split}$$

Generalizations of Theorem 1 to the semilinear case, $F \neq 0$, requires much more involved arguments. The challenge is to obtain the same order of convergence $\frac{1}{2}$, when considering test functions of class C^2 with bounded first and second order derivatives. Two strategies which have been used to prove the generalizations are explained below – each for one type of discretization only, but both approaches apply for temporal and spatial discretization.

4.2. The semilinear case: space-discretization, Poisson equation approach. Reference: [4].

Main tool: Poisson equation. Generalization in the infinite dimensional case of [15]. Used for stochastic nonlinear Schrödinger equations in [12].

Assume that $L_F < \lambda_1$: there exists unique invariant distributions μ_{∞} (exact problem) and μ_{∞}^N , for $N \in \mathbb{N}$. Moreover, convergence to equilibrium is exponentially fast, with a uniform rate with respect to $N \in \mathbb{N}$.

The presentation is simpler than in the mentioned references, in particular we do not introduce time-averages, we directly focus at error at equilibrium. Note also that we skip some technical details, such as auxiliary spectral Galerkin approximation to justify the use of the objects in the infinite dimensional setting.

Introduce the notation

$$\overline{\varphi} = \varphi - \int \varphi d\mu_{\infty}.$$

The associated Poisson equation is

$$\mathcal{L}\Psi = -\overline{\varphi} , \quad \int \Psi d\mu_{\infty} = 0,$$

with the infinitesimal generator

$$\mathcal{L}\phi(x) = \langle Ax + F(x), D\phi(x) \rangle + \operatorname{Tr}(D^2\phi(x)),$$

for appropriate functions $\phi : H \to \mathbb{R}$: in order to give meaning to all the terms in the expression of $\mathcal{L}\phi(x)$, assuming ϕ of class \mathcal{C}^2 is not sufficient.

Let us first explain why the solution Ψ of the Poisson equation is useful.

On the one hand, the error may be written

$$\int \varphi d\mu_{\infty}^{N} - \int \varphi d\mu_{\infty} = \int \overline{\varphi} d\mu_{\infty}^{N} = -\int \mathcal{L}\Psi d\mu_{\infty}^{N}$$
$$= -\int \left(\langle Ax + F(x), D\Psi(x) \rangle + \operatorname{Tr} \left(D^{2}\Psi(x) \right) \right) d\mu_{\infty}^{N}(x).$$

On the other hand, since μ_{∞}^N is the unique invariant distribution for X^N ,

$$0 = \int \mathcal{L}_N(\Psi \circ P_N) d\mu_\infty^N = \int \left(\langle Ax + P_N F(x), D\Psi(x) \rangle + \operatorname{Tr} \left(P_N D^2 \Psi(x) \right) \right) d\mu_\infty^N(x),$$

where \mathcal{L}_N is the infinitesimal generator for the (SDE) evolution of X^N .

Thus, summing the two equations, the error has the following expression:

$$\int \varphi d\mu_{\infty}^{N} - \int \varphi d\mu_{\infty} = \int \langle (P_{N} - I)F(x), D\Psi(x) \rangle d\mu_{\infty}^{N}(x) + \int \operatorname{Tr} \left((P_{N} - I)D^{2}\Psi(x) \right) d\mu_{\infty}^{N}(x).$$

To obtain rates of convergence, estimates on the derivatives of Ψ are required. They are of the following type:

$$|(-A)^{\alpha}D\Psi(x)| \le C_{\alpha} \quad , \quad ||(-A)^{\beta}D^{2}\Psi(x)(-A)^{\gamma}||_{\mathcal{L}(H)} \le C_{\beta,\gamma},$$

equivalently, in terms of differentials,

$$D\Psi(x).((-A)^{\alpha}h) \le C_{\alpha}|h| \quad , \quad D^{2}\Psi(x).((-A)^{\beta}h_{1}, (-A)^{\gamma}h_{2}) \le C_{\beta,\gamma}|h_{1}||h_{2}|,$$

with a range for values of α, β, γ made precise below.

With such estimates, error terms are controlled as follows, using $||(I - P_N)(-A)^{-\alpha}||_{\mathcal{L}(H)} \leq \frac{C_{\alpha}}{\lambda_N^{\alpha}}$, equivalently $|(I - P_N)x| \leq \frac{C_{\alpha}}{\lambda_N^{\alpha}}|(-A)^{\alpha}x|$.

First,

$$\left| \int \langle (P_N - I)F(x), D\Psi(x) \rangle d\mu_{\infty}^N(x) \right| \le C \| (I - P_N)(-A)^{-\alpha} \|_{\mathcal{L}(H)} \sup_{x \in H} |(-A)^{\alpha} D\Psi(x)|.$$

Second,

$$\left|\int \operatorname{Tr}\left((P_N - I)D^2\Psi(x)\right)d\mu_{\infty}^N(x)\right| \le C_{\beta,\gamma}\operatorname{Tr}\left((-A)^{-\frac{1}{2}-\kappa}\right)\|(I - P_N)(-A)^{\frac{1}{2}+\kappa-\beta-\gamma}\|_{\mathcal{L}(H)}$$
$$\times \sup_{x\in H}\|(-A)^{\beta}D^2\Psi(x)(-A)^{\gamma}\|_{\mathcal{L}(H)}.$$

To get order of convergence $\frac{1}{2} - \kappa$, it remains to prove that we are allowed to choose $\alpha = \beta = \gamma = \frac{1}{2} - \kappa$ in the estimates of derivatives of Ψ .

Now, let us discuss well-posedness and properties of the solution Ψ of the Poisson equation. In fact, note that $\overline{\varphi}$ solves the centering condition $\int \overline{\varphi} d\mu_{\infty} = 0$, thus the function

$$\Psi(x) = -\int_0^\infty \mathbb{E}\big[\overline{\varphi}(X(t,x))\big]dt$$

is well-defined. Let $\overline{u}(t,x) = \mathbb{E}\left[\overline{\varphi}(X(t,x))\right]$. Indeed, thanks to the exponential convergence estimate, $\left|\overline{u}(t,x)\right| \leq C(\varphi,|x|)e^{-(\lambda_1-L_F)t}$.

It is possible to check that (up to finite dimensional approximations to justify the expressions and computations, with bounds independent of the dimension)

• $\overline{u}(t, \cdot)$ is of class \mathcal{C}^2 , for any $t \ge 0$,

• the spatial derivatives satisfy, for t > 0,

 $|(-A)^{\alpha}D\overline{u}(t,x)| \le C_{\alpha}t^{-\alpha}e^{-ct} \quad , \quad ||(-A)^{\beta}D^{2}\overline{u}(t,x)(-A)^{\gamma}||_{\mathcal{L}(H)} \le C_{\beta,\gamma}t^{-\beta-\gamma}e^{-ct},$

with c > 0, for $\alpha \in [0, 1)$ and $\beta, \gamma \in [0, 1)$ such that $\beta + \gamma < 1$,

• \overline{u} solves the Kolmogorov equation

$$\frac{\partial \overline{u}(t,x)}{\partial t} = \mathcal{L}\overline{u}(t,x) , t > 0, x \in H.$$

with initial condition $\overline{u}(0, \cdot) = \overline{\varphi}$,

- $\Psi = -\int_0^\infty \overline{u}(t,\cdot)dt$ solves the Poisson equation $\mathcal{L}\Psi = \overline{\varphi}$ with $\int \Psi d\mu_\infty = 0$,
- the derivatives of Ψ satisfy

$$|(-A)^{\alpha}D\Psi(x)| \le C_{\alpha} \quad , \quad ||(-A)^{\beta}D^{2}\Psi(x)(-A)^{\gamma}||_{\mathcal{L}(H)} \le C_{\beta,\gamma},$$

for $\alpha \in [0, 1)$ and $\beta, \gamma \in [0, 1)$ such that $\beta + \gamma < 1$.

The estimates on the spatial derivatives of \overline{u} may be interpreted as a regularization property: indeed, at time t = 0, $\overline{u}(0, \cdot) = \overline{\varphi}$ is only assumed of class C^2 , and to satisfy the estimate only for $\alpha = \beta = \gamma = 0$. At positive times t > 0 (and, after integration, for Ψ), positive values of $\alpha, \beta, \gamma > 0$ can be chosen, with singularities $t^{-\alpha}, t^{-\beta}, t^{-\gamma}$ in the estimates.

4.3. The semilinear case: time-discretization, Kolmogorov equation approach. Reference: [1].

Main tool: Kolmogorov equation. Generalization in the infinite dimensional case of [16] (for instance). Used for stochastic nonlinear Schrödinger equations in [6].

We will not give lots of details, in particular because controlling some of the error terms requires tools such as Malliavin integration by parts.

The idea is to control the weak error

$$\left|\mathbb{E}\varphi(X_n^{\Delta t}) - \mathbb{E}\varphi(X(n\Delta t))\right|$$

and to prove upper bounds which do not depend on $t = n\Delta t$, *i.e.* of the type $C_{\kappa} \|\varphi\|_2 \Delta t^{\frac{1}{2}-\kappa}$. Letting $t = n\Delta t \to \infty$ then yield a control of

$$\big|\int \varphi d\mu_{\infty}^{\Delta t} - \int \varphi d\mu_{\infty}.$$

The expansion of the error uses the solution u of the (infinite dimensional) Kolmogorov equation

$$\frac{\partial u(t,x)}{\partial t} = \mathcal{L}u(t,x) , t > 0, x \in H.$$

with initial condition $u(0, \cdot) = \varphi$.

Indeed, the weak error may be expanded as follows,

$$\mathbb{E}\varphi(X_n^{\Delta t}) - \mathbb{E}\varphi(X(n\Delta t)) = \mathbb{E}u(0, X_n^{\Delta t}) - \mathbb{E}u(n\Delta t, X_0^{\Delta t})$$
$$= \sum_{k=0}^{n-1} \mathbb{E}\left[u\left((n-1-k)\Delta t, X_{k+1}^{\Delta t}\right) - u\left((n-k)\Delta t, X_k^{\Delta t}\right)\right]$$
$$= \sum_{k=0}^{n-1} (a_k + b_k + c_k)$$

with

$$a_{k} = \int_{k\Delta t}^{(k+1)\Delta t} \mathbb{E} \langle AS_{\Delta t}X_{k}^{\Delta t} - A\tilde{X}^{\Delta t}(t), Du(n\Delta t - t, \tilde{X}^{\Delta t}(t)) \rangle dt,$$

$$b_{k} = \int_{k\Delta t}^{(k+1)\Delta t} \mathbb{E} \langle S_{\Delta t}F(X_{k}^{\Delta t}) - F(\tilde{X}^{\Delta t}(t)), Du(n\Delta t - t, \tilde{X}^{\Delta t}(t)) \rangle dt,$$

$$c_{k} = \int_{k\Delta t}^{(k+1)\Delta t} \mathbb{E} \mathrm{Tr} \Big((S_{\Delta t}^{2} - I) D^{2}u(n\Delta t - t, \tilde{X}^{\Delta t}(t)) \Big) dt$$

where the auxiliary process satisfies $\tilde{X}^{\Delta t}(k\Delta t) = X_k^{\Delta t}$ (interpolation) and evolves through

$$d\tilde{X}^{\Delta t}(t) = AS_{\Delta t}X_k^{\Delta t}dt + S_{\Delta t}F(X_k^{\Delta t})dt + \sqrt{2}S_{\Delta t}dW(t) , \quad t \in (k\Delta t, (k+1)\Delta t).$$

Similarly to the analysis of the spectral Galerkin discretization, the key inequality to obtain order of convergence is

$$\|(S_{\Delta t} - I)(-A)^{-\alpha}\|_{\mathcal{L}(H)} \le C_{\alpha} \Delta t^{\alpha}.$$

And estimates of the type

$$|(-A)^{\alpha} Du(t,x)| \le C_{\alpha} t^{-\alpha} e^{-ct} \quad , \quad ||(-A)^{\beta} D^{2} u(t,x)(-A)^{\gamma}||_{\mathcal{L}(H)} \le C_{\beta,\gamma} t^{-\beta-\gamma} e^{-ct}$$

with rate c > 0, are required – in order to consider the regime $n\Delta t \to \infty$. They are satisfied with $\alpha = \beta = \gamma = \frac{1}{2} - \kappa$. The control of the terms a_k, b_k is not trivial. Indeed, naive estimates are obtained using

The control of the terms a_k, b_k is not trivial. Indeed, naive estimates are obtained using Hölder regularity estimates with exponent $\frac{1}{4} - \kappa$: but they only yield an order of convergence $\frac{1}{4} - \kappa$, instead of $\frac{1}{2} - \kappa$. The solution, following [10], is to use a Malliavin integration by parts, to replace some stochastic integrals. We do not give more details in these lecture notes.

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