

PDE Approaches for the Long-Time Behavior of Diffusion Processes

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This note is dedicated to the long-time behavior of diffusion processes via PDE approaches.

1 Theory of hypocoercivity

1.1 From Langevin dynamics to $L = A^*A + B$

Let \mathcal{H} be a separable Hilbert space. The theory of hypocoercivity [1] is to study diffusion processes with generator in the form

$$L = A^*A + B, \quad (1.1)$$

where A, B are two unbounded operator in \mathcal{H} and B is anti-symmetric, i.e., $B = -B^*$. For such an operator, its kernel \mathcal{K} (a subset of \mathcal{H}) is characterized by $\mathcal{K} = \ker(A) \cap \ker(B)$. Also, an important property of the operator L is the semigroup e^{-tL} is a contraction, i.e., $\|e^{-tL}\| \leq 1, \forall t \geq 0$.

Usually, the Hilbert space \mathcal{H} is chosen to be $L^2(\mu_\infty)$, where μ_∞ is the equilibrium of a given diffusion process. Also, $A = (A_1, \dots, A_m)$ and B are usually in the form

$$A_j h = a_j \cdot \nabla h, \quad B h = b \cdot \nabla h.$$

Here, h is usually the probability density with respect to μ_∞ . Let ρ_∞ be the probability density of μ_∞ with respect to the Lebesgue measure. If we compactly write $Ah = \sigma \nabla h$, where σ is an $m \times n$ matrix, then we have

1. $B = -B^* \iff \nabla \cdot (b\rho) = 0$;
2. $A^*g = -\nabla \cdot (\sigma^*g) - \langle \nabla \rho_\infty, \sigma^*g \rangle$.

Therefore, for a given diffusion process, we may try to derive the operator $L = A^*A + B$ in the following steps:

1. Find the unique invariant distribution μ_∞ .
2. Rewrite the Fokker-Planck equation in terms of the probability density with respect to μ_∞ .
3. Determine the operator A according to the second-order part.
4. Determine the operator B according to the remaining part.

Now we present two examples of diffusion processes and derive the operator L in the $A^*A + B$ form.

1.1.1 Overdamped Langevin dynamics

The overdamped Langevin dynamics in \mathbb{R}^n is given by

$$dX_t = \sqrt{2}\sigma(X_t)dW_t + \xi(X_t)dt, \quad (1.2)$$

where $\xi \in C^1(\mathbb{R}^n; \mathbb{R}^n)$ is the drift function, and $\sigma \in C^2(\mathbb{R}^n; \mathbb{R}^{n \times m})$ is the diffusion coefficient, and W_t is the standard Wiener process in \mathbb{R}^m . The corresponding Fokker–Planck equation is

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D \nabla \rho - \xi \rho), \quad D = \sigma^* \sigma. \quad (1.3)$$

Suppose the process admits a unique invariant distribution $\mu_\infty(dx) = \rho_\infty(x)dx$ (determined by ξ and σ), then the probability density $h(t, x) = \rho(t, x)/\rho_\infty$ satisfies the diffusion equation

$$\frac{\partial h}{\partial t} = \nabla \cdot (D \nabla h) - \left(\xi - 2D \nabla \log \rho_\infty \right) \cdot \nabla h. \quad (1.4)$$

Hence the operator L in $L^2(\mu_\infty)$ is given by $L = A^*A + B$, where the operators A, B are given by

$$\boxed{A = \sigma \nabla, \quad B = (\xi - 2D \nabla \log \rho_\infty) \cdot \nabla.} \quad (1.5)$$

When the diffusion matrix D is non-degenerate, the kernel space \mathcal{K} consists of constant functions.

1.1.2 Underdamped Langevin dynamics

The underdamped Langevin dynamics in \mathbb{R}^n is given by

$$\begin{cases} dX_t = V_t, \\ dV_t = -V_t - \nabla V(X_t) + \sqrt{2}dW_t, \end{cases} \quad (1.6)$$

where $V \in C^1(\mathbb{R}^n; \mathbb{R})$ is the potential function. When $V(x)$ satisfies the confinement condition, the unique invariant distribution μ_∞ is given by the density function

$$\rho_\infty(x, v) = \frac{1}{Z} \exp \left(-V(x) - \frac{|v|^2}{2} \right). \quad (1.7)$$

The Fokker–Planck equation is

$$\frac{\partial \rho}{\partial t} + v \cdot \nabla_x \rho - \nabla V(x) \cdot \nabla_v \rho = \Delta_v \rho + \nabla_v \cdot (v f). \quad (1.8)$$

The probability density $h(t, x, v) = \rho(t, x, v)/\rho_\infty$ then satisfies

$$\frac{\partial h}{\partial t} + v \cdot \nabla_x h - \nabla V(x) \cdot \nabla_v h = \Delta_v h - v \cdot \nabla_v h. \quad (1.9)$$

Hence the operator L in $L^2(\mu_\infty)$ is given by $L = A^*A + B$, where the operators A, B are given by

$$\boxed{A = \nabla_v, \quad B = v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v.} \quad (1.10)$$

The kernel space \mathcal{K} consists of constant functions.

1.2 Hypocoercivity theorem

1.2.1 Basic theorem

We present the basic theorem of the hypocoercivity. It is based on the assumption that both A and A^* commute with $[A, B]$.

Theorem 1.1 *Consider the linear operator $L = A^*A + B$ where B is anti-symmetric. Let $C = [A, B]$ be the commutator. If there exist constant α, β such that*

1. A and A^* commute with C ;
2. $[A, A^*]$ is α -bounded to I and A ;
3. $[B, C]$ is β -bounded to A, A^2, C and AC .

Then there is a scalar product $((\cdot, \cdot))$ on $\mathcal{H}^1/\mathcal{K}$ such that

$$((h, Lh)) \geq K(\|Ah\|^2 + \|Ch\|^2) \quad (1.11)$$

for some $K > 0$ which only depends on α and β .

Here, the norm in the Hilbert space \mathcal{H}^1 is defined by

$$\|h\|_{\mathcal{H}^1}^2 = \|h\|^2 + \|Ah\|^2 + \|Ch\|^2, \quad (1.12)$$

which is the counterpart of the Sobolev space.

Proof In the proof, the scalar product $((\cdot, \cdot))$ is explicitly chosen as

$$((h, g)) = \langle h, g \rangle + a\langle Ah, Ag \rangle + b\Re\langle Ah, Ch \rangle + b\Re\langle Ag, Ch \rangle + c\langle Ch, Ch \rangle. \quad (1.13)$$

In particular, when $h = g$,

$$((h, h)) = \|h\|^2 + a\|Ah\|^2 + 2b\Re\langle Ah, Ch \rangle + c\|Ch\|^2. \quad (1.14)$$

Note that the commutation between A, C allows the norm defined above makes sense. This norm is equivalent to \mathcal{H}^1 . The rate of change for the $((\cdot, \cdot))$ norm of $e^{-tL}h$ is

$$-\frac{1}{2} \frac{d}{dt} ((e^{-tL}h, e^{-tL}h)) = \Re((e^{-tL}h, e^{-tL}Lh)). \quad (1.15)$$

By direct calculation, we have the estimate

$$\begin{aligned} \Re((h, Lh)) &\geq \|Ah\|^2 \\ &+ a \left(\|A^2h\|^2 - \|Ah\| \| [A, A^*] Ah \| - \|Ah\| \|Ch\| \right) \\ &+ \left(\|Ch\|^2 - \|Ah\| \|R_2h\| - 2\|A^2h\| \|CAh\| - \|Ch\| \| [A, A^*] Ah \| \right) \\ &+ \left(\|CAh\|^2 - \|Ch\| \|R_2h\| \right). \end{aligned}$$

As a consequence, we have

$$\Re((h, Lh)) \geq \langle X, mX \rangle_{\mathbb{R}^4}, \quad (1.16)$$

where X is the vector $(\|Ah\|, \|A^2h\|, \|Ch\|, \|CAh\|)$, and the 4×4 matrix m is given by

$$m = \begin{bmatrix} 1 - (a\alpha + b\beta) & -(a\alpha + b\beta) & -(a + b\alpha + b\beta + c\beta) & -b\beta \\ 0 & a & -(b\alpha + c\beta) & -2b \\ 0 & 0 & b - c\beta & -c\beta \\ 0 & 0 & 0 & c \end{bmatrix}. \quad (1.17)$$

With appropriate choices of the parameters a, b, c , one may ensure that the symmetric part of m is positive definite, and hence the theorem holds true. \square

We present a simple example that the conditions of the basic theorem hold true. Consider the underdamped Langevin dynamics, where the operators A, B are given by

$$A = \nabla_v, \quad B = v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v. \quad (1.18)$$

Recall that the density of the invariant distribution is

$$\rho_\infty(x, v) = \frac{1}{Z} \exp\left(-V(x) - \frac{|v|^2}{2}\right). \quad (1.19)$$

Then the adjoint operator A^* satisfies $A^*h = -\nabla_v(\rho_\infty h)$, and we have

$$\begin{aligned} ABh &= \nabla_v(v \cdot \nabla_x h - \nabla V(x) \cdot \nabla_v h) \\ &= \nabla_x h + v \cdot \nabla_{xh}^2 h - \nabla V(x) \cdot \nabla_v^2 h, \\ BAh &= v \cdot \nabla_x(\nabla_v h) - \nabla V(x) \cdot \nabla_v(\nabla_v h) \\ &= v \cdot \nabla_{xh}^2 h - \nabla V(x) \cdot \nabla_v^2 h. \end{aligned}$$

Therefore, the commutator C is explicitly given by $C = AB - BA = \nabla_x$, which commutes with A and A^* . Therefore, the basic theorem can be applied to the underdamped Langevin dynamics.

In this case, the kernel space \mathcal{K} consists of constant functions, and norm in the Hilbert space \mathcal{H}^1 is defined by

$$\|h\|_{\mathcal{H}^1}^2 = \|h\|^2 + \|\nabla_x h\|^2 + \|\nabla_v h\|^2. \quad (1.20)$$

Therefore, \mathcal{H}^1 is the usual H^1 space corresponding to the probability measure μ_∞ , while \mathcal{H} itself is the usual L^2 space. Then we have the hypocoercivity

$$\|e^{-tL}\|_{\mathcal{H}^1/\mathcal{K}} \leq Ce^{-\lambda t} \quad (1.21)$$

for some constants $C, \lambda > 0$.

1.2.2 Generalized theorem

The generalized theorem of hypocoercivity allows a sequence of commutators.

Theorem 1.2 *Let \mathcal{H} be a Hilbert space, and $A : \mathcal{H} \rightarrow \mathcal{H}^n$ and $B : \mathcal{H} \rightarrow \mathcal{H}$ be unbounded operators with $B^* = -B$. Let $L = A^*A + B$ and $\mathcal{K} := \ker L$. Assume there exists $N_c \in \mathbb{N}$ and operators $\{C_j\}_{j=0}^{N_c+1}$ and $\{R_j\}_{j=0}^{N_c+1}$ such that*

$$C_0 = A, \quad [C_j, B] = Z_{j+1}C_{j+1} + R_{j+1}, \quad C_{N_c+1} = 0. \quad (1.22)$$

And for $k \in \{0, 1, \dots, N_c\}$,

1. $[A, C_k]$ is bounded relatively to $\{C_j\}_{j=0}^k$ and $\{C_j A\}_{j=0}^{k-1}$;
2. $[C_k, A^*]$ is bounded relatively to I and $\{C_j\}_{j=0}^k$;
3. R_k is bounded relatively to $\{C_j\}_{j=0}^{k-1}$ and $\{C_j A\}_{j=0}^{k-1}$;
4. There are positive constants λ_j, Λ_j such that $\lambda_j I \leq Z_j \leq \Lambda_j$.

Then there is a scalar product $((\cdot, \cdot))$ on \mathcal{H}^1 , which defines a norm equivalent to the \mathcal{H}^1 norm

$$\|h\|_{\mathcal{H}^1}^2 = \|h\|^2 + \sum_{j=0}^{N_c} \|C_j h\|^2 \quad (1.23)$$

such that

$$\Re((h, Lh)) \geq K \sum_{j=0}^{N_c} \|C_j h\|^2, \quad \forall h \in \mathcal{H}^1/\mathcal{K}. \quad (1.24)$$

We note that each C_j consists of the high-order terms of A and B . After some commutator operations, the high-order terms vanish in C_{N_c+1} .

The proof is accomplished by defining the norm

$$((h, h)) = \|h\|^2 + \sum_{k=0}^{N_c} \left(a_k \|C_k h\|^2 + 2\Re b_k \langle C_k h, C_{k+1} h \rangle \right) \quad (1.25)$$

and choosing the constants a_k and b_k carefully.

1.2.3 Entropic convergence theorem

The entropic convergence theorem requires the operators A, B to be exactly the first-order differential operators.

Theorem 1.3 *Let $E \in C^2(\mathbb{R}^N)$ such that e^{-E} is rapidly decreasing and $\mu(X) = e^{-E(X)} dX$ is a probability measure on \mathbb{R}^N . Let $(A_j)_{1 \leq j \leq m}$ and B be first-order derivation operators with smooth coefficients. Denote A_j^* and B^* by their respective adjoints in $L^2(\mu)$, and assume $B = -B^*$. Denote A by the collection (A_1, \dots, A_m) and define*

$$L = A^* A + B = \sum_{j=1}^m A_j^* A_j + B. \quad (1.26)$$

Assume there exists $N \in \mathbb{N}_c$, derivation operators $C_0, C_1, \dots, C_{N_c+1}$, R_1, \dots, R_{N_c+1} and vector-valued functions Z_1, \dots, Z_{N_c+1} such that

$$C_0 = A, \quad [C_j, B] = Z_{j+1} C_{j+1} + R_{j+1}, \quad (0 \leq j \leq N_c), \quad C_{N_c+1} = 0, \quad (1.27)$$

and

1. $[A, C_k]$ is pointwise bounded to A ;
2. $[C_k, A^*]$ is pointwise bounded to $I, \{C_j\}_{0 \leq j \leq k}$;
3. R_k is pointwise bounded to $\{C_j\}_{0 \leq j \leq k-1}$;

4. There are positive constants λ_j, Λ_j such that $\lambda_j \leq Z_j \leq \Lambda_j$;
5. $[A, C_k]^*$ is pointwise bounded to I, A .

Then there exists a quadratic form S in \mathbb{R}^N such that the functional

$$\mathcal{E}(h) = \int h \log h d\mu + \int \frac{\langle S \nabla h, \nabla h \rangle}{h} d\mu \quad (1.28)$$

satisfies

$$\frac{d}{dt} \mathcal{E}(e^{-tL} h) \leq -\alpha \int \frac{\langle S \nabla h, \nabla h \rangle}{h} d\mu. \quad (1.29)$$

In the proof, the functional \mathcal{E} is chosen to be the form

$$\mathcal{E}(h) = \int f u + \sum_{k=0}^{N_c} \left(a_k \int f |C_k u|^2 + 2b_k \int f \langle C_k u, C_{k+1} u \rangle \right), \quad (1.30)$$

where a_k, b_k are the parameters to be determined.

2 Generalized Γ calculus for the long-time behavior

The generalized Γ calculus was developed in [2] to study the long-time behavior of a wide class of stochastic processes. It extends the classical Bakry–Emery theory and applies to the degenerate diffusion processes.

2.1 Generalized Γ calculus

Consider a stochastic process in \mathbb{R}^d with generator L . For any differential real value functional Φ , define the Γ operator by

$$\Gamma_\Phi(f) = \frac{1}{2} (L\Phi(f) - d\Phi(f).Lf), \quad (2.1)$$

where the test function is smooth in \mathbb{R}^d and $d\Phi(f)$ is understood as

$$d\Phi(f).g = \lim_{s \rightarrow 0} \frac{\Phi(f + sg) - \Phi(f)}{s}. \quad (2.2)$$

The generalized Γ function recovers the classical carré du champ operator in the following way:

- If $\Phi(f) = |f|^2$, then $\Gamma_\Phi(f) = \Gamma(f) = \frac{1}{2} (L(f^2) - 2fLf)$ is the classical Γ operator.

By direct calculation, for $\Phi(f) = |f|^2$ we have

$$d\Phi(f).g = \lim_{s \rightarrow 0} \frac{|f + sg|^2 - |f|^2}{s} = 2fg. \quad (2.3)$$

Introduce the bilinear form corresponding to the Γ operator by

$$\Gamma(f, g) = \frac{1}{2} (L(fg) - fLg - gLf), \quad (2.4)$$

then the Γ operator is simply written as $\Gamma(f) = \Gamma(f, f)$.

- If $\Phi(f) = \Gamma(f)$, then $\Gamma_\Phi(f) = \Gamma_2(f) = \frac{1}{2}(L\Gamma(f) - 2\Gamma(f, Lf))$ is the classical Γ_2 operator.

By direct calculation, for $\Phi(f) = \Gamma(f)$ we have

$$\begin{aligned} d\Phi(f).g &= \lim_{s \rightarrow 0} \frac{\Gamma(f + sg) - \Gamma(f)}{s} \\ &= \lim_{s \rightarrow 0} \left(L(fg) + \frac{s}{2}L(g^2) - (fLg + gLf) - sgLg \right) \\ &= 2\Gamma(f, g). \end{aligned}$$

Hence $\Gamma_\Phi(f) = \Gamma_2(f) = \frac{1}{2}(L\Gamma(f) - 2\Gamma(f, Lf))$. It is also convenient to extend Γ_2 to

$$\Gamma_2(f, g) = \frac{1}{2}(L\Gamma(f, g) - \Gamma(f, Lg) - \Gamma(g, Lf)). \quad (2.5)$$

- If $\Phi(f) = a(f)$ for some scalar function a , then $\Gamma_\Phi(f) = \frac{1}{2}(L(a(f)) - a'(f)Lf)$.

By direct calculation,

$$d\Phi(f).g = a'(f)g.$$

Hence $\Gamma_\Phi(f) = \frac{1}{2}(L(a(f)) - a'(f)Lf)$. If L contains the derivation operator $b(x) \cdot \nabla_x$, then it vanishes in the expression of $\Gamma_\Phi(f)$. If L contains the diffusion operator Δ and the scalar function $a(r) = r \log r$, then it is easy to check $\Gamma_\Phi(f) = |\nabla f|^2/f$.

The Γ function is important because it represents the rate of change for the observable functions. Suppose the stochastic process has the semigroup $(P_t)_{t \geq 0}$, and define the observable function by

$$\psi(s) = P_s \Phi(P_{t-s}f)(x), \quad (2.6)$$

then $\psi'(s) = 2P_s \Gamma_\Phi P_{t-s}f(x)$. Therefore, for a given function Φ , the curvature condition naturally reveals the long-time behavior of the semigroup $(P_t)_{t \geq 0}$.

Lemma 2.1 *Given the differentiable real value functional Φ . The curvature condition $\Gamma_\Phi \geq \rho\Phi$ for some $\rho \in \mathbb{R}$, is equivalent to the*

$$\Phi(P_t f) \leq e^{-2\rho t} \Phi_t(f), \quad \forall f \geq 0. \quad (2.7)$$

Note the operator P_t is positivity preserving. Also, the Γ operator is linear in the function Φ , and Φ should be nonlinear for Γ to make sense.

We say a scalar function $a \in C^4$ is admissible if a is strictly convex and $1/a''$ is concave. For an admissible function, introduce the a -entropy by

$$\text{Ent}_\nu^a(f) = \nu(a(f)) - a(\nu f) \geq 0. \quad (2.8)$$

The a -entropy is equivalent when a is added by a constant. The most common choice of a is $a(r) = r \log r$ with $a''(r) = 1/r$, and the resulting a -entropy is the classical relative entropy. The following lemma estimates Γ_Φ for a specific form of Φ .

Lemma 2.2 *If L is a diffusion operator, C is a linear operator, $a : \mathbb{R}^+ \rightarrow \mathbb{R}$ is an admissible function such that $\Phi(f) = a''(f)|Cf|^2$, then*

$$\Gamma_\Phi(f) \geq a''(f)Cf.[L, C]f. \quad (2.9)$$

The proof only used the fact that $\alpha = 1/a''$ is concave.

The following lemma makes use of the curvature condition to prove the exponential convergence.

Lemma 2.3 *Suppose the semigroup $(P_t)_{t \geq 0}$ is ergodic with an invariant distribution μ ,*

$$0 \leq \int \Phi_1(f) d\mu - \Phi_1\left(\int f d\mu\right) \leq c \int \Phi_2(f) d\mu, \quad \forall f \geq 0, \quad (2.10)$$

and $\Gamma_{\Phi_2} \geq \rho\Phi_2 - \beta\Gamma_{\Phi_1}$ for some $\beta > 0$, then the function

$$W(t) = \beta \left(\int \Phi_1(P_t f) d\mu - \Phi_1\left(\int f d\mu\right) \right) + \int \Phi_2(P_t f) d\mu \quad (2.11)$$

satisfies $W(t) \leq e^{-\frac{2\rho t}{1+\beta c}} W(0)$. In particular,

$$\int \Phi_2(P_t f) d\mu \leq (1 + \beta c) e^{-\frac{2\rho t}{1+\beta c}} \int \Phi_2(f) d\mu. \quad (2.12)$$

2.2 Underdamped Langevin dynamics

For the underdamped Langevin dynamics, the infinitesimal generator L (not the one used in the hypocoercivity) is given by

$$Lf(x, y) = \left[y \cdot \nabla_x - \left(y + \nabla_x U \right) \cdot \nabla_y + \Delta_y \right] f(x, y). \quad (2.13)$$

The invariant distribution of the dynamics is

$$\mu(dx dy) = \frac{1}{Z} \exp \left(-U(x) - \frac{|y|^2}{2} \right). \quad (2.14)$$

Choose the functions $\Phi_1(f) = f \log f$ and

$$\Phi_2(f) = \frac{|(\nabla_x - \nabla_y)f|^2 + |\nabla_y f|^2}{f}, \quad (2.15)$$

then $\Gamma_{\Phi_1}(f) = |\nabla_y f|^2/f$. For the choices of Φ_1, Φ_2 , we have

$$\bullet \quad 0 \leq \int \Phi_1(f) d\mu - \Phi_1\left(\int f d\mu\right) \leq c \int \Phi_2(f) d\mu.$$

In fact, this is equivalent to the log-Sobolev inequality

$$\text{Ent}_\mu(f) \leq c \int \frac{|\nabla f|^2}{f} d\mu, \quad (2.16)$$

which holds true due to the classical Bakry–Emery theory.

$$\bullet \quad \Gamma_{\Phi_2} \geq \rho\Phi_2 - \beta\Gamma_{\Phi_1}.$$

In Lemma 2.2, choose $\Phi_{2a} = |(\nabla_x - \nabla_y)f|^2/f$ and $\Phi_{2b} = |\nabla_y f|^2$, we have

$$\Gamma_{\Phi_{2a}} \geq \frac{(\nabla_y - \nabla_x)f \cdot (\nabla_y - \nabla_x - \nabla_x^2 U \nabla_y)f}{f}, \quad (2.17)$$

$$\Gamma_{\Phi_{2b}} \geq \frac{\nabla_y f \cdot (\nabla_y - \nabla_x)f}{f}. \quad (2.18)$$

Hence

$$\Gamma_{\Phi_2} = \Gamma_{\Phi_{2a}} + \Gamma_{\Phi_{2b}} \geq \frac{p|(\nabla_y - \nabla_x)f|^2 - q|\nabla_y f|^2}{f} = p\Phi_2(f) - (p+q)\Gamma_{\Phi_1}. \quad (2.19)$$

The two conditions above imply that the result of Lemma 2.3 holds true. That is, there is exponential convergence in the sense of Φ_2 . More precisely,

$$\text{Ent}_\mu(P_t f) \leq e^{-\lambda t} \left(\frac{3}{\beta} \int \frac{|\nabla f|^2}{f} d\mu + \text{Ent}_\mu(f) \right). \quad (2.20)$$

The generalized curvature condition $\Gamma_{\Phi_2} \geq \rho\Phi_2 - \beta\Gamma_{\Phi_1}$ plays an important role in the proof.

References

- [1] Cédric Villani. Hypocoercivity. *arXiv preprint math/0609050*, 2006.
- [2] Pierre Monmarché. Generalized γ calculus and application to interacting particles on a graph. *Potential Analysis*, 50(3):439–466, 2019.