MATHEMATIK

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Hypocoercivity of Langevin-type dynamics on abstract manifolds

An Application to fibre lay-down models

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Motivation

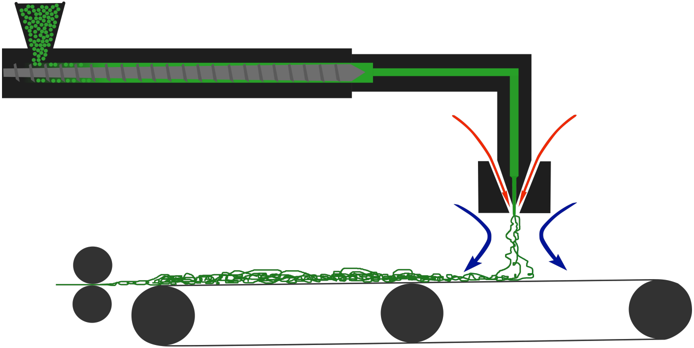

Figure 1: Melt blow production process

- We use Langevin-type fibre lay-down models as surrogate models.
- We want to analyse the convergence to equilibrium state and hope for exponential decay with explicitly computable rates:
  ‚The faster the convergence the more uniform the nonwoven material.'

Motivation

More formally: Let $(T_t)_{t\in[0,\infty)}$ the corresponding Langevin semigroup on the abstract model Hilbert space H. There are explicitly computable constants κ_1 and κ_2 such that

$$\|T_t g - (g\,,1)_H\|_H \leq \kappa_1 \mathrm{e}^{-\kappa_2 t}\,\|g-(g\,,1)_H\|_H \qquad \text{for all times } t\geq 0$$

and for all $g \in H$.

- Pioneering work by Villani.
- For linear kinetic equations by Dolbeault, Mouhot and Schmeiser ('09, '15) for an abstract Hilbert space setting under assumptions (D) and (H).
- Grothaus and Stilgenbauer ('14, '16) taking all domain issues into account.

Classical Langevin equation

Problem (Purely Euclidean case)

By the term classical Langevin equation we refer to the Stratonovich SDE

$$\begin{aligned} \mathrm{d}x_t &= v_t \, \mathrm{d}t \\ \mathrm{d}v_t &= -\nabla\Psi(x_t)\, \mathrm{d}t + \sigma \circ \mathrm{d}W_t - \alpha \cdot v_t \, \mathrm{d}t, \end{aligned} \tag{1}$$

with positions $x_t \in \mathbb{R}^d_x$, velocities $v_t \in \mathbb{R}^d_v$, potential Ψ on $\mathbb{R}^d_x$, fircition parameter $\alpha \in (0, \infty)$ and diffusion parameter $\sigma \in (0, \infty)$.
The Kolmogorov backward generator reads as

$$L = \frac{\sigma^2}{2}\,\Delta_v - \alpha \cdot (v \,, \nabla_v)_{\mathrm{euc}} + (v \,, \nabla_x)_{\mathrm{euc}} - (\nabla_x \Psi \,, \nabla_v)_{\mathrm{euc}}.$$

For fibre lay-down applications we would replace $\mathbb{R}^d_v$ by the sphere $\mathbb{S}^{d-1}_v$.
Grothaus and Stilgenbauer established the hypocoercivity result for $\mathbb{R}^d_x$ and both cases of velocity spaces.

Classical Langevin equation

Questions

1. smooth side condition on position:
   Replace $\mathbb{R}_x^d$ by an abstract manifold $\mathbb{M}$:
   - How does the Langevin equation (1) change?
   - How does the generator L change?
   - Does the hypocoercivity method still apply?
2. (algebraic) side condition on velocity:
   Additionally, we demand that $|v_t|^2 = 1$; how do answers from above change? What about other (algebraic) side conditions?

Hypocoercivity method

- Data conditions (D): model Hilbert space $H = L^2(Q;\mu)$, invariant measure μ for L, decomposition $L = S - A$ on some core D for L, existence of a strongly continuous semigroup $(T_t)_{t\in[0,\infty)}$, suitable projections P_S and P with $P_S = P + (\cdot\,,1)_H$, conservativity
- Hypocoercivity conditions (H): e. g.
  - microscopic coercivity:
    $\exists\,\Lambda_m \in (0,\infty)\,\forall\, f \in D\colon\ \Lambda_m \|(\mathrm{Id} - P_S)f\|_H^2 \le -(Sf\,,f)_H$
  - macroscopic coercivity:
    $\exists\,\Lambda_M \in (0,\infty)\,\forall\, f \in D\big((AP)^*(AP)\big)\colon\ \Lambda_M \|Pf\|_H^2 \le \|APf\|_H^2$
- Potential conditions (P): Poincaré inequality for the measure $\exp(-\Psi)\,\lambda_{\mathrm{m}}$ on $\mathbb{M}$, boundedness from below, (weak) regularity assumptions

Example

Consider the classical Langevin equation (1). Then, $D = C_c^\infty(\mathbb{R}_x^d \times \mathbb{R}_v^d)$ and $S = \frac{\sigma^2}{2}\,\Delta_v - \alpha\cdot(v\,,\nabla_v)_{\mathrm{euc}}$ as well as $A = -(v\,,\nabla_x)_{\mathrm{euc}} + (\nabla_x\Psi\,,\nabla_v)_{\mathrm{euc}}$.
Also, $\mu = \exp(-\Psi)\lambda \otimes \nu_0$ for some zero-mean Gaussian measure ν_0.

How to set up the SDE?

Things laying around, but do not fit perfectly:

- Itô-type approach in the Itô-bundle (Gliklikh)
- Stratonovich-type approach and horizontal diffusions in the frame bundle (e. g. Ikeda-Watanabe, Hackenbroch-Thalmaier, Hsu etc.)
- stochastic Hamiltonian systems (Kolokoltsov)
- misc.: stochastic action integrals, jet bundle formalism, Hilbert complexes, hypoelliptic Laplacians (Bismut) etc.

We choose kind of a ‚Lagrangian' approach relying on

1. the enhanced McKean-Gangolli injection scheme as elaborated by Jørgensen (1977),
2. an Ehresmann connection and the associated semispray (e. g. Bucataru).

Influences of geometry

Let an m-dimensional, real, connected Riemannian manifold $(\mathbb{M}, \mathrm{m})$ be geodesically complete/complete as metric space.

- An orientation on $\mathbb{M}$ is not needed.
- Without assuming parallelisability the tangent bundle $\mathrm{T}\mathbb{M}$ (or smooth sub-fibre bundles) just has an almost product structure, i. e. we can not globally think an element as tupel (x, v).
  - Instead of a product measures on $\mathrm{T}\mathbb{M}$ we use 'almost product measures' exploiting local triviality. I. e. for probability measures $\mu_{\mathbb{M}}$ on $\mathbb{M}$ and ν_0 on $\mathbb{R}^m$ there is a probability measure $\mu_{\mathbb{M}} \otimes_{\mathrm{loc}} \nu_0$ on $\mathrm{T}\mathbb{M}$ locally looking like $\mu_{\mathbb{M}} \otimes \nu$.
  - Expressions like $\mathrm{m}(v\,,\nabla_v f)$ or $\mathrm{m}(\nabla_x \Psi\,,\nabla_v f)$ make no sense; there is no such thing as $\nabla_x f$ and in particular, $\mathrm{m}(v\,,\nabla_x f)$ is not defined, $f \in C^\infty(\mathrm{T}\mathbb{M})$.

Almost product structure of fibre bundles

Definition (fibre bundle)

A smooth mapping $\pi\colon \mathbb{E} \to \mathbb{B}$ between manifolds is called *fibre bundle with (standard) fibre F* if it satisfies the property of local trivialisation: For any $x \in \mathbb{B}$ there is an open neighbourhood $U_x \subseteq \mathbb{B}$ as well as a diffeomorphism φ rendering the diagram in Figure 2 commutative.

$$\begin{array}{ccc} \pi^{-1}(U_x) & \xrightarrow{\varphi} & U_x \times F \\ {\scriptstyle \pi}\downarrow & \swarrow {\scriptstyle \mathrm{pr}_1} & \\ U_x & & \end{array}$$

Figure 2: Local trivialisation of a fibre bundle

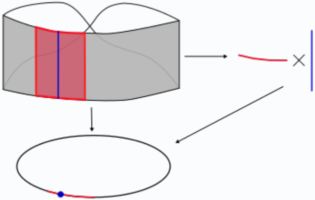

Figure 3: Generic example with Möbius strip as total space

We are interested in two common instances which do not trivialise globally:

Example

- tangent bundles: $\pi_0\colon \mathrm{T}\mathbb{M} \to \mathbb{M}$, $\pi_0(v) = x$ for all $v \in \mathrm{T}_x\mathbb{M}$, $F = \mathbb{R}^m$, exponentially weighted base measure $\exp(-\Psi)\lambda_{\mathrm{m}}$, Gaussian fibre measure (not in this talk)
- unit tangent bundles: $\pi_0\colon \mathrm{S}\mathbb{M} \to \mathbb{M}$, $F = \mathbb{S}^{m-1}$, exponentially weighted base measure $\mu_{\mathbb{M}} := \exp(-\Psi)\lambda_{\mathrm{m}}$, normalised surface measure ν as fibre measure (no friction term)

Local product measures like $\mu_{\mathbb{M}} \otimes_{\mathrm{loc}} \nu$ on $\mathrm{S}\mathbb{M}$ are constructed in a trivialisation as pushforward of $\mu_{\mathbb{M}} \otimes \nu$ wrt. φ^{-1}.

Ehresmann connections

Definition (vertical vectors and lift)

The space of *vertical* vectors $\mathrm{VT}\mathbb{M} := \mathrm{Null}(d\pi_0)$; we understand $a \in \mathrm{VT}\mathbb{M}$ as being tangent to the fibre $\pi_0^{-1}(\{\pi_1(a)\})$, where π_1 is the projection in the double tangent bundle $\mathrm{TT}\mathbb{M} \to \mathbb{M}$.
There is a canonical identification of $\mathrm{V}_v\mathrm{T}\mathbb{M}$ and $\mathrm{T}_x\mathbb{M}$ for all $v \in \mathrm{T}\mathbb{M}$, $x := \pi_0(v)$: The *vertical lift at v* $\mathrm{vl}_v\colon\ \mathrm{T}_x\mathbb{M} \to \mathrm{V}_v\mathrm{T}\mathbb{M}$ is characterised by its action on functions $f \in C^\infty(\mathbb{M})$ as $\langle \mathrm{vl}_v(w)\,, d_v(df)\rangle = \langle w\,, df\rangle$.

Definition (Ehresmann connection)

An *Ehresmann connection* is a decomposition $\mathrm{TT}\mathbb{M} = \mathrm{VT}\mathbb{M} \oplus \mathrm{HT}\mathbb{M}$ in sense of a Whitney sum. Vectors in $\mathrm{HT}\mathbb{M}$ are said to be ‘horizontal’.

There is no canonical Ehresmann connection in the first place. Via the corresponding exponential mapping a Riemannian metric does induce an Ehresmann connection which in turn corresponds to the Levi-Civita connection. This one will be fixed.

Ehresmann connections and semisprays

Definition (horizontal lift)

Consider an Ehresmann connection. For all $v, w \in \mathrm{T}\mathbb{M}$ the *horizontal lift of w at v* is the unique vector $\mathrm{hl}_v(w) \in \mathrm{H}_v\mathrm{T}\mathbb{M}$ such that

$$w = \langle \mathrm{hl}_v(w)\,,\, d\pi_0 \rangle.$$

Definition (semispray)

A section $\mathcal{H} \in \Gamma^\infty(\mathrm{T}\mathbb{M}; \mathrm{TT}\mathbb{M})$ is a *semispray* if it satisfies $\langle \mathcal{H}\,,\, d\pi_0 \rangle = \mathrm{Id}_{\mathrm{T}\mathbb{M}}$. Equivalently, any integral curve $s\colon \mathbb{I} \to \mathrm{T}\mathbb{M}$ satisfies $(\pi_0 \circ s)' = s$. A curve $c\colon \mathbb{I} \to \mathbb{M}$ is a *geodesic of $\mathcal{H}$* if $c = \pi_0 \circ s$ for some integral curve s.

So, an Ehresmann connection induces a semispray via $\mathcal{H}(w) := \mathrm{hl}_w(w)$. All in all, there is the so-called *Riemannian semispray $\mathcal{H}_\mathrm{m}$* induced by the Riemannian metric m on $\mathbb{M}$.

Notes on the Riemannian semispray

Remark

- The maximal flow of $\mathcal{H}_{\mathrm{m}}$ is the geodesic flow. Thus, $\mathcal{H}_{\mathrm{m}}$ often goes by the name geodesic spray.
- The Lagrangian vector field corresponding to the Lagrangian $\mathrm{T}\mathbb{M} \to \mathbb{R}$, $v \mapsto \frac{1}{2}\,\mathrm{m}(v\,,v)$ is exactly $\mathcal{H}_{\mathrm{m}}$.
- If a function $f \in C^\infty(\mathrm{T}\mathbb{M})$ can be written as $f = f_0 \circ \pi_0$ for some $f_0 \in C^\infty(\mathbb{M})$, then the semispray $\mathcal{H}_{\mathrm{m}}$ acts on f as

$$\mathcal{H}_{\mathrm{m}} f = \mathrm{m}_{\pi_0}(\mathrm{Id}_{\mathrm{T}\mathbb{M}}\,, \nabla_{\mathrm{m}} f_0 \circ \pi_0).$$

If $\mathbb{M} = \mathbb{R}^m_x$ is endowed with Euclidean Riemann metric, then we have for every function $f\colon\ \mathbb{R}^m_x \times \mathbb{R}^m_v \to \mathbb{R}$, $(x, v) \mapsto f_0(x)$ that

$$\mathcal{H}_{\mathrm{euc}} f(x, v) = (v\,, \nabla_x f_0(x))_{\mathrm{euc}} \qquad \text{for all } x, v \in \mathbb{R}^m.$$

Sasaki metric

Definition (Sasaki metric)

The *Sasaki metric* s is the unique Riemannian metric on $\mathbb{TM}$ respecting the given Ehresmann connection:

$$\mathrm{s}(\mathsf{vl}\,\mathcal{X},\mathsf{vl}\,\mathcal{Y}) = \mathrm{m}(\mathcal{X},\mathcal{Y}), \quad \mathrm{s}(\mathsf{hl}\,\mathcal{X},\mathsf{hl}\,\mathcal{Y}) = \mathrm{m}(\mathcal{X},\mathcal{Y}),$$

$$\text{and} \qquad \mathrm{s}(\mathsf{vl}\,\mathcal{X},\mathsf{hl}\,\mathcal{Y}) = 0$$

for all vector fields $\mathcal{X},\mathcal{Y} \in \Gamma^\infty(\mathbb{M};\mathbb{TM})$.

The Sasaki metric splits into a 'vertical metric' and a 'horizontal metric': $\mathrm{s} = \mathrm{v} + \mathrm{h}$. Similarly, the Sasakian gradient splits into a 'vertical gradient' and a 'horizontal gradient': $\nabla_\mathrm{s} = \nabla_\mathrm{v} + \nabla_\mathrm{h}$. Intuitively, we think this as $\nabla_\mathrm{v} \approx \nabla_v$ and $\nabla_\mathrm{h} \approx \nabla_x$!

What do we do now?

- Consider the unit tangent bundle $\mathbb{SM} \leq \mathbb{TM}$ as configuration manifold Q encoding the algebraic side condition $|v|_{\mathrm{m}}^2 = \mathrm{m}(v\,,\,v) = 1$. I. e. a solution would be a curve $\eta\colon\ \mathbb{I} \to \mathsf{Q}$ with $\mathbb{I}$ a time interval.
- The unit tangent bundle basically inherits its Ehresmann connection from the tangent bundle. However, the vertical lift to $\mathrm{V}\mathbb{TM}$ needs to be adapted to yield a lift to $\mathrm{V}\mathbb{SM}$ indeed. This lift is denoted by tl as it is unfortunately called 'tangent lift':

$$\mathrm{T}\mathbb{TM}|_{\mathbb{SM}} = \mathrm{T}\mathbb{SM} \oplus \mathrm{N}\mathbb{SM} = \mathsf{tl}(\mathbb{SM}) \oplus \mathrm{H}\mathbb{TM}|_{\mathbb{SM}} \oplus \mathrm{N}\mathbb{SM}.$$

  The vertical gradient ∇_{v} is to be modified too yielding the spherical gradient $\nabla_{\mathbb{S}}$ etc.
- The symmetric operator S will be ‚vertical'; the antisymmetric operator A will be minus the Riemannian semispray up to a correction term. In mathematical physics, operators of the form of $-A$ describe geodesic motion of a particle on $\mathbb{M}$ in presence of a potential field.

The fibre lay-down model over $\mathbb{M}$

The classical system (1) now is reformulated on $\mathrm{Q} = \mathbb{SM}$ as

$$\mathrm{d}\eta = \mathcal{H}_{\mathrm{m}}\,\mathrm{d}t + \mathsf{tl}_\eta(-\nabla_{\mathrm{m}}\Psi)\,\mathrm{d}t + \sigma \cdot \mathsf{tl}_\eta\left(\sum_{j=1}^{m} \frac{\partial}{\partial x_\eta^j}\right) \circ \mathrm{d}W_t, \qquad (2)$$

where the chart $\left(x_\eta^1, x_\eta^2, \ldots, x_\eta^m\right)$ at $\pi_0(\eta) \in \mathbb{M}$ provides normal coordinates. The generator has the form

$$L = \frac{\sigma^2}{2}\,\Delta_{\mathbb{S}} + \underbrace{\mathcal{H}_{\mathrm{m}} - \mathsf{tl}(\nabla_{\mathrm{m}}\Psi)}_{=:-A} =: S - A,$$

where the spherical Laplace-Beltrami $\Delta_{\mathbb{S}}$ is the natural modification of the vertical Laplace-Beltrami Δ_{v} acting on functions from $C^\infty(\mathbb{SM})$.

Check the data assumptions

We choose the model Hilbert space $H := L^2(\mathrm{Q};\mu) = L^2(\mathbb{SM};\mu)$ with $\mu := \exp(-\Psi)\lambda_{\mathrm{m}} \otimes_{\mathrm{loc}} \nu$, where ν is the uniform measure on the fibre $\mathbb{S}^{m-1}$.

Lemma (*SAD*-decomposition of the generator L)

Let the potential Ψ be loc-Lipschitzian such that

$$\mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0) = (m-1)\,\Psi^{\mathrm{h}} \qquad \text{on } \mathbb{SM}, \tag{3}$$

where Ψ^{h} is the horizontal lift of Ψ, i. e. $(\mathrm{tl}\,\mathcal{X})\Psi^{\mathrm{h}} = (\mathcal{X}\Psi) \circ \pi_0$ holds for all $\mathcal{X} \in \Gamma^\infty(\mathbb{M};\mathrm{Q})$.
Then, we have $L = S - A$ on $D = C_c^\infty(\mathbb{SM})$ such that

1. $(S, D) = \left(\frac{\sigma^2}{2}\Delta_{\mathbb{S}}, C_c^\infty(\mathbb{SM})\right)$ *is symmetric,*
2. $(A, D) = (-\mathcal{H}_{\mathrm{m}} + \mathrm{tl}(\nabla_{\mathrm{m}}\Psi), C_c^\infty(\mathbb{SM}))$ *is antisymmetric, and*
3. *for all $f \in D$ we have that $Lf \in L^1(\mathbb{SM};\mu)$ with $\int_{\mathbb{SM}} Lf \,\mathrm{d}\mu = 0$.*

Note that assumption (3) always is fulfilled for $\mathbb{M} = \mathbb{R}^m_x$.

Proof

1. Wlog. $\sigma^2 = \sqrt{2}$. Using 'vertical' integration by parts we immediately get that $S = \Delta_{\mathbb{S}}$ generates the spherical gradient form which reads on the predomain $D = C_c^\infty(\mathrm{S}\mathbb{M})$ as $\mathcal{E}_{\mathbb{S}}(f, g) := \int_{\mathrm{S}\mathbb{M}} \mathrm{v}(\nabla_{\mathbb{S}} f\ , \nabla_{\mathbb{S}} g)\ \mathrm{d}\mu$.
2. This is tricky! With the assumption (3) $\mathrm{tl}(\nabla_{\mathrm{m}}\Psi)$ transforms to $\frac{1}{m-1}\nabla_{\mathbb{S}}(\mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0))$. Looks worse, but it's actually the desired correction term: The adjoint operator $((-\mathcal{H}_{\mathrm{m}})^*, D)$ wrt. $L^2(\mathrm{Q}; \mu)$-scalar product is $(-\mathcal{H}_{\mathrm{m}})^* = \mathcal{H}_{\mathrm{m}} - \mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0)$ by Liouville's Theorem. The adjoint operator $(\mathrm{tl}(\nabla_{\mathrm{m}}\Psi)^*, D)$ wrt. $L^2(\mathrm{Q}; \mu)$-scalar product can be computed as

$$\left(\frac{1}{m-1}\,\nabla_{\mathbb{S}}(\mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0))\right)^*$$
$$= -\frac{1}{m-1}\,\nabla_{\mathbb{S}}(\mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0)) - \frac{1}{m-1}\,\Delta_{\mathbb{S}}(\mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0))$$
$$= -\frac{1}{m-1}\,\nabla_{\mathbb{S}}(\mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0)) + \mathcal{H}_{\mathrm{m}}(\Psi \circ \pi_0).$$

3. Clear, when combining the previous results.

Conclusion

- We found a suitable model to transfer results just known in case of Euclidean position space.
- We proved that the hypocoercivity method applies to the Langevin-type fibre lay-down model:
  - under weak geometric assumptions on $\mathbb{M}$ (finite-dimensional, connected, geodesically complete)
  - for a large class of potentials Ψ (loc-Lipschitzian, bounded from below, assumption (3), Poincaré inequality of $\exp(-\Psi)\lambda_{\mathrm{m}}$)
- In principle, we are able to incorporate other (algebraic) side conditions on the velocity by choosing Q as another smooth sub-fibre bundle of the tangent bundle. However, we just dealt with the case of Q being boundaryless.

Selected references on the hypocoercivity method

- J. Dolbeault, C. Mouhot, C. Schmeiser, Hypocoercivity for kinetic equations with linear relaxation terms, C. R. Acad. Sci. Paris **347**, 511-516 (2009).
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- M. Grothaus, P. Stilgenbauer, Hilbert space hypocoercivity for the Langevin dynamics revisited, Methods Funct. Anal. Topology **22**, 152-168 (2016).

Thank you for your attention!

Are there any questions?