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Optimal non-symmetric Fokker-Planck equation for the convergence to a given equilibrium

Anton ARNOLD

with Christian Schmeiser, Beatrice Signorello

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Topic & goals

symmetric Fokker-Planck equation for $f(x,t)$:

- $$f_t = \text{div}(\nabla f + f\nabla V(x)), \quad x \in \mathbb{R}^d,\ t > 0$$

  $\rightarrow$ Decay estimate to $f_\infty(x) = c_V e^{-V(x)}$ with rate $\inf_x \lambda_{min}(\frac{\partial^2 V}{\partial x^2})$ by entropy method (Bakry-Emery strategy)
- This rate is sharp for $V(x) = \frac{x^T \mathbf{K}^{-1} x}{2}$, $\mathbf{K} > 0$,
  $f_\infty(x) = c_{\mathbf{K}} e^{-V(x)}$ ... anisotropic Gaussian

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Theme:

- Non-symmetric perturbations of the drift (that preserve f_∞) can enhance the convergence.
- Goal: Find optimal perturbation that yields best exponential estimate

  $$\|f(t) - f_\infty\|_{L^2(f_\infty^{-1})} \le c\, e^{-\lambda t} \|f_0 - f_\infty\|_{L^2(f_\infty^{-1})}, \quad t \ge 0,$$

  with (1) maximal $\lambda > 0$ and (2) minimal $c \ge 1$.

stochastic applications

- compute expectations w.r.t. measure $\mu_V = e^{-V}dx$ (high dimensions)

$\rightarrow$ needs to construct an ergodic Markov process with fast convergence to the unique measure μ_V.

References:

- Lelièvre-Nier-Pavliotis: *Optimal non-reversible linear drift for the convergence to equilibrium of a diffusion, J. Stat. Phys., 2013*
- *Guillin-Monmarché: Optimal linear drift for the speed of convergence of an hypoelliptic diffusion, Electron. Commun. Probab., 2016*

Outline:

1. Fokker-Planck equations with linear drift: propagator norm
2. construction of best (hypocoercive) Fokker-Planck equations
3. numerical illustrations
4. outlook: Fokker-Planck equations with t-dependent coefficients

degenerate Fokker-Planck equations with linear drift

$$f_t \;=\; \operatorname{div}\Big(\mathbf{D}\nabla f + \mathbf{C}x\, f\Big) =: -Lf\,, \quad x \in \mathbb{R}^d \tag{1}$$

with degenerate $0 \le \mathbf{D} = \mathbf{D}^T \in \mathbb{R}^{d\times d}$ is degenerate parabolic;
(symmetric part of) L is not coercive.

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Definition 1 (Villani 2009)

Consider L on Hilbert space H with $\mathcal{K} = \ker L$; let $\tilde{H} \hookrightarrow \mathcal{K}^\perp$ (densely)
(e.g. H ... weighted L^2, $\tilde{H}$ ... weighted H^1).
L is called hypocoercive on $\tilde{H}$ if $\exists\, \lambda > 0,\ c \ge 1$:

$$\|e^{-Lt} f_0\|_{\tilde{H}} \le c\, e^{-\lambda t}\|f_0\|_{\tilde{H}} \qquad \forall\, f_0 \in \tilde{H}$$

- typically $c > 1$

hypocoercive Fokker-Planck equation

$$f_t = \operatorname{div}\Big(\mathbf{D}\,\nabla f + \mathbf{C}\,x\,f\Big) =: -Lf\,, \quad x \in \mathbb{R}^d \tag{2}$$

Condition A:

1. No (nontrivial) subspace of $\ker \mathbf{D}$ is invariant under $\mathbf{C}^\top$.
   (equivalent: L is hypoelliptic.)
2. Let $\mathbf{C} \in \mathbb{R}^{d\times d}$ be positive stable (i.e. $\Re(\lambda^{\mathbf{C}}) > 0$).
   [$\Rightarrow \exists$ confinement potential; drift towards $x = 0$.]

- hypoelliptic + confinement = hypocoercive (for FP eq.)

hypocoercive Fokker-Planck equation

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- hypoelliptic + confinement = hypocoercive (for FP eq.)

Lemma 1

Let Condition A *hold. Then:*

- (2) *is hypocoercive.*
- $f_\infty(x) = c_{\mathbf{K}} \exp\left(-\frac{x^T\mathbf{K}^{-1}x}{2}\right)$ *is the unique steady state, with* $\mathbf{K} = \mathbf{K}^T > 0$ *solves* $2\mathbf{D} = \mathbf{CK} + \mathbf{KC}^T$ *(continu. Lyapunov eq. for* $\mathbf{K}$*)*

normalization of Fokker-Planck equations

original FP-equation: $$f_t = \text{div}\left(\mathbf{D}\,\nabla_x f + \mathbf{C}\,x\,f\right) =: -Lf\,,\;\; x\in\mathbb{R}^d$$

coordinate transformation: $y := \mathbf{K}^{-1/2}x,\;\; g(y) := \sqrt{\det(\mathbf{K})}\,f(\mathbf{K}^{1/2}y)\;\;\Rightarrow$

normalized FP-equation: $$g_t = \text{div}\left(\tilde{\mathbf{D}}\,\nabla_y g + \tilde{\mathbf{C}}\,y\,g\right) =: -\tilde{L}g\,,\;\; y\in\mathbb{R}^d$$

corresponding drift-ODE: $\frac{d}{dt}y(t) = -\tilde{\mathbf{C}}y(t),\quad \tilde{\mathbf{C}} := \mathbf{K}^{-1/2}\mathbf{C}\mathbf{K}^{1/2}$

with $\tilde{\mathbf{D}} = \mathbf{K}^{-1/2}\mathbf{D}\mathbf{K}^{-1/2}\quad\Rightarrow\quad \tilde{\mathbf{D}} = \tilde{\mathbf{C}}_s \geq 0$

Then $g_\infty(x) = (2\pi)^{-d/2}e^{-|y|^2/2}$.

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Then $g_\infty(x) = (2\pi)^{-d/2}e^{-|y|^2/2}$.

L^2–propagator norm ($\to$ our main tool):

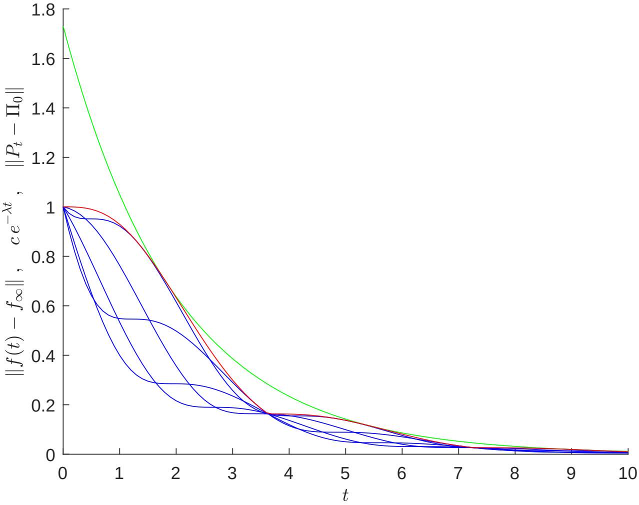
Theorem 2 (AA-Schmeiser-Signorello, CMS 2022)

Let Condition A *hold. Then:*

$$\left\|e^{-Lt}\right\|_{\mathcal{B}(\{f_\infty\}^\perp)} = \left\|e^{-\tilde{L}t}\right\|_{\mathcal{B}(\{g_\infty\}^\perp)} = \left\|e^{-\tilde{\mathbf{C}}t}\right\|_{\mathcal{B}(\mathbb{R}^d)}, \qquad \forall t \geq 0$$

L^2–propagator norm

propagator norm of Fokker-Planck equ. in 2D: $\|e^{-Lt} - \Pi_0\|_{\mathcal{B}(L^2(f_\infty^{-1}))}$



Proof of Theorem 2; for normalized FP (step 1)

Theorem 3

Let $\tilde{L} = -\operatorname{div}\left(\tilde{\mathbf{D}}\,\nabla\cdot + \tilde{\mathbf{C}}\,y\,\cdot\right)$ *satisfy Condition A (i.e.* $\tilde{L}$ *is hypocoercive). Then*

$$\|e^{-\tilde{L}t} - \tilde{\Pi}_0\|_{\mathcal{B}(\mathcal{H})} = \|e^{-\tilde{\mathbf{C}}t}\|_2, \quad t \geq 0.$$

$\tilde{\Pi}_0$ ... *projection on* $\operatorname{span}[g_\infty]$, $g_\infty = c\, e^{-|y|^2/2}$

- $\tilde{L}$ ... non-symmetric. Still, $\exists$ a partially orthogonal decomposition:

$$\mathcal{H} := L^2(g_\infty^{-1}) = \bigoplus_{m\in\mathbb{N}_0}^{\perp} V^{(m)}; \quad V^{(m)} = \operatorname{span}[g_\alpha(y) := (-1)^{|\alpha|}\nabla^\alpha g_\infty,\ |\alpha| = m]$$

$$\sigma(L) = \left\{\sum_{j=1}^{d} \alpha_j \lambda_j,\ \alpha \in \mathbb{N}_0^d\right\}; \quad \lambda_j \ldots \text{eigenvalues of } \tilde{\mathbf{C}} \in \mathbb{R}^{d\times d}$$

Proof (step 2): evolution in subspaces $V^{(m)}$

$d_\alpha(t)$ ... coefficient of $g_\alpha(y)$, $\alpha \in \mathbb{N}_0^d$, $y \in \mathbb{R}^d$

<u>ex. $d = 2$:</u>

- $m = 1$: $\frac{\mathrm{d}}{\mathrm{d}t}\binom{d_{(1,0)}}{d_{(0,1)}} = -\tilde{\mathbf{C}}\binom{d_{(1,0)}}{d_{(0,1)}}$ ... drift-ODE

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- $m = 2$: $\begin{pmatrix} d_{(2,0)} \\ d_{(1,1)} \\ d_{(0,2)} \end{pmatrix}$ ... impractical !

  better: $D^{(2)}(t) := \begin{pmatrix} d_{(2,0)} & d_{(1,1)}/2 \\ d_{(1,1)}/2 & d_{(0,2)} \end{pmatrix}(t) \in \mathbb{R}^{2\times 2}$

$$\frac{\mathrm{d}}{\mathrm{d}t} D^{(2)} = -(\tilde{\mathbf{C}} D^{(2)} + D^{(2)} \tilde{\mathbf{C}}^T)$$

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- $m \geq 3$: $D^{(m)}(t)$ ... symmetric m-order tensor

$$\frac{\mathrm{d}}{\mathrm{d}t} D^{(m)}(t) = -m\,\mathrm{Sym}\big(\underbrace{\tilde{\mathbf{C}} \odot D^{(m)}(t)}_{\text{mult. on 1st index}}\big)$$ ... tensored drift-ODE

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$\Rightarrow$ FP = 2nd quantization of ODE in Bosonic Fock space of $\mathbb{R}^2$

Proof (step 3): evolution in subspaces $V^{(m)}$

• practical ingredient for estimating the evolution equation in $V^{(m)}$: rank-1 decomposition of order-m tensors:

$$D^{(m)} = \sum_{k=1}^{s} \mu_k v_k^{\otimes m}, \quad \mu_k \in \mathbb{R},\ v_k \in \mathbb{R}^d \tag{3}$$

minimal s: "symmetric rank" of $D^{(m)}$

Lemma 2

Let (3) be the decomposition of $D^{(m)}(0)$. Then, the evolution in $V^{(m)}$ is given by

$$D^{(m)}(t) = \sum_{k=1}^{s} \mu_k [v_k(t)]^{\otimes m}, \quad \dot{v}_k = -\tilde{\mathbf{C}} v_k \ .$$

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- subspaces $V^{(m)}$ are orthogonal
- decay behavior of $\|e^{-\tilde{L}t} - \tilde{\Pi}_0\|_{\mathcal{B}(\mathcal{H})}$ determined only by 1^{st} subspace

  $\rightarrow$ equivalent to drift-ODE: $\|e^{-\tilde{\mathbf{C}}t}\|_2$

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(non-normalized) Fokker-Planck equations with linear drift

Let steady state $f_{\infty,K}(x) = \frac{\det(\mathbf{K})^{-1/2}}{(2\pi)^{-d/2}} \exp\left(-\frac{x^T\mathbf{K}^{-1}x}{2}\right)$, $\mathbf{K} > 0$ be given.

$$\text{Find} \qquad f_t = \operatorname{div}(\mathbf{D}\nabla f + \mathbf{C}xf) =: -L_{C,D}f \quad \text{with fastest decay;} \qquad (4)$$

diffusion matrix $\mathbf{D} \geq 0$; drift matrix $\mathbf{C}$: positive stable, i.e. $\Re(\lambda^{\mathbf{C}}) > 0$.

admissible matrices: $\mathcal{I}(\mathbf{K}) := \left\{(\mathbf{C}, \mathbf{D}) : \mathbf{D} \geq 0,\ \mathrm{Tr}\,(\mathbf{D}) \leq d,\ L_{C,D}f_{\infty,K} = 0\right\}$

- Without constraint $\mathrm{Tr}\,(\mathbf{D}) \leq d$ arbitrary decay possible $\rightarrow$ ill-posed.

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Lemma 3 (Guillin-Monmarché 2016)

$$\mathcal{I}(\mathbf{K}) = \left\{\mathbf{D} \geq 0,\ \mathrm{Tr}\,(\mathbf{D}) \leq d;\ \mathbf{C} = (\mathbf{D}+\mathbf{J})\mathbf{K}^{-1},\ \mathbf{J}^T = -\mathbf{J}\right\}.$$

Lemma 4

Let $\mathbf{K} > 0$, $(\mathbf{C},\mathbf{D}) \in \mathcal{I}(\mathbf{K})$, $\mathbf{C}$ *positive stable.*
Then $f_{\infty,K}$ *is the unique (normalized) steady state; (4) is hypocoercive.*

Questions

hypocoercivity: $$\|f(t)-f_{\infty,K}\|_{L^2(f_{\infty,K}^{-1})} \le c\, e^{-\lambda t}\|f_0-f_{\infty,K}\|_{L^2(f_{\infty,K}^{-1})}, \quad t\ge 0 \tag{5}$$

1. Which FP-evolutions converge the fastest, i.e. with largest rate λ_{opt} to the steady state in the operator norm of $e^{-L_{C,D}t}$ on $\{f_{\infty,K}\}^\perp \subset \mathcal{H} := L^2(\mathbb{R}^d, f_{\infty,K}^{-1})$?
2. When the best decay rate is fixed, what is the infimum of the multiplicative constant, c_{inf}, in the decay estimate (5)?
3. For a fixed $\mathbf{K} > 0$ and the corresponding λ_{opt}, and for any $c > c_{inf}$, which pair(s) of matrices $(\mathbf{C}_{opt}(c), \mathbf{D}_{opt}(c) \ge 0)$ yields the convergence estimate (5) with the constants (λ_{opt}, c)?
4. For such an optimal pair of matrices, what bound on $\|\mathbf{C}_{opt}\|$ can be found, and how does this bound grow w.r.t. to the space dimension d?

Results from the literature

Lemma 5 (Guillin-Monmarché 2016)

- *Question Q1:* $\lambda_{opt} = \lambda_{max}(\mathbf{K}^{-1})$.
- *Question Q2: They can only reach multiplicative constants* $c > \sqrt{\kappa(\mathbf{K})\, e}$.
- *Questions Q3+Q4: Their drift matrix grows like* $\|\mathbf{C}_{opt}\| = \mathcal{O}(d^2)$ *(with piecewise constant coefficients).*

$\kappa(\mathbf{K})$ ... condition number

Strategy for improvement

non-symmetric FP-equation: $f_t = \mathrm{div}(\mathbf{D}\nabla f + \mathbf{C}xf) =: -L_{C,D} f$

corresponding drift-ODE: $\frac{d}{dt} y(t) = -\tilde{\mathbf{C}} y(t), \quad \tilde{\mathbf{C}} := \mathbf{K}^{-1/2}\mathbf{C}\mathbf{K}^{1/2}$

Main tool:

Theorem 4 (AA-Schmeiser-Signorello, CMS 2022)

Let $\mathbf{K} > 0$, $(\mathbf{C}, \mathbf{D}) \in \mathcal{I}(\mathbf{K})$, $\mathbf{C}$ *positive stable. Then:*

$$\left\| e^{-L_{C,D} t} \right\|_{\mathcal{B}(\{f_{\infty,K}\}^{\perp})} = \left\| e^{-\tilde{\mathbf{C}} t} \right\|_{\mathcal{B}(\mathbb{R}^d)}, \qquad \forall t \geq 0,$$

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- This reduces the PDE-optimization problem to an ODE-problem, and allows for sharp result.
- Replacing a hypocoercive entropy method used in [Guillin-Monmarché 2016]; block-diagonal decomposition of the FP-propagator used in [Lelièvre-Nier-Pavliotis 2013].

Main result: optimal constants

Theorem 5 (AA-Signorello 2021)

Let $\mathbf{K} > 0$ *be given. Then:*

(a) *Questions Q2+Q3:* $c_{inf} = 1$. *For any constant* $c > 1$, *there exists a pair* $(\mathbf{C}_{opt}(c), \mathbf{D}_{opt}(c)) \in \mathcal{I}(\mathbf{K})$ *such that*

$$\left|\left| e^{-L_{C_{opt},D_{opt}} t} \right|\right|_{\mathcal{B}(V_0^\perp)} \leq c\, e^{-\max(\sigma(\mathbf{K}^{-1}))t}, \qquad t \geq 0. \tag{6}$$

(b) *Question Q4: The matrices from (a) satisfy*

$$||\mathbf{C}_{opt}||_{\mathcal{F}} \leq \lambda_{opt} \left[d + \sqrt{\kappa(\mathbf{K})}\, \frac{2\pi c^2}{\sqrt{3}(c^2-1)}\, \sqrt{d}\, (d-1) \right], \quad ||\mathbf{D}_{opt}||_{\mathcal{F}} = d. \tag{7}$$

$||\mathbf{C}||_{\mathcal{F}}$ ... Frobenius norm

Proof-idea (refinement of [Lelièvre-Nier-Pavliotis 2013], [Guillin-Monmarché 2016])

1. normalize FP-equation: $y := \mathbf{K}^{-1/2}x$

$$\Rightarrow g_t = \operatorname{div}(\tilde{\mathbf{D}}\nabla g + \tilde{\mathbf{C}}yg), \quad g_\infty(y) = (2\pi)^{-d/2}e^{-|y|^2/2}, \quad y \in \mathbb{R}^d,$$

with $\tilde{\mathbf{D}} := \mathbf{K}^{-1/2}\mathbf{D}\mathbf{K}^{-1/2} \geq 0$, $\tilde{\mathbf{J}} := \mathbf{K}^{-1/2}\mathbf{J}\mathbf{K}^{-1/2} = -\tilde{\mathbf{J}}^T$,
$\tilde{\mathbf{C}} := \mathbf{K}^{-1/2}\mathbf{C}\mathbf{K}^{1/2} = \tilde{\mathbf{D}} + \tilde{\mathbf{J}}$.

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2. Construction of $\mathbf{D}$:
   Maximal decay rate of $e^{-\tilde{\mathbf{C}}t}$, $\lambda_{opt} = \lambda_{max}(\mathbf{K}^{-1})$ only possible if
   $\operatorname{ran}(\mathbf{D}) \subset \text{eigenspace}_{\lambda_{max}}(\mathbf{K}^{-1})$;
   e.g. $\mathbf{D} := d\, v \otimes v$ (with $\mathbf{K}^{-1}v = \lambda_{opt}v$, $\|v\| = 1$) ... rank 1.

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1. normalize FP-equation: $y := \mathbf{K}^{-1/2}x$

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   e.g. $\mathbf{D} := d\, v \otimes v$ (with $\mathbf{K}^{-1}v = \lambda_{opt}v$, $\|v\| = 1$) ... rank 1.

3. $\exists$ algorithmic construction of $\tilde{\mathbf{J}}$, $\mathbf{P} > 0$ such that:

$$\mathbf{P}\underbrace{(\tilde{\mathbf{D}} + \tilde{\mathbf{J}})}_{=\tilde{\mathbf{C}}} + \underbrace{(\tilde{\mathbf{D}} - \tilde{\mathbf{J}})}_{=\tilde{\mathbf{C}}^T}\mathbf{P} = 2\lambda_{opt}\mathbf{P}$$ ... continuous Lyapunov equation for $\mathbf{P}$

Proof-idea (cont'd)

4. decay of drift-ODE $\dot{y}(t) = -\tilde{\mathbf{C}}y(t)$ in norm $\|y\|_{\mathbf{P}}^2 := \langle y, \mathbf{P}y\rangle$:

$$\frac{d}{dt}\|y(t)\|_{\mathbf{P}}^2 = -\langle y(t), [\mathbf{P}\tilde{\mathbf{C}} + \tilde{\mathbf{C}}^T\mathbf{P}]y(t)\rangle = -2\lambda_{opt}\|y(t)\|_{\mathbf{P}}^2.$$

$$\Rightarrow \quad \|y(t)\|_{\mathbf{P}} = e^{-\lambda_{opt} t}\|y(0)\|_{\mathbf{P}}, \qquad t \geq 0.$$

Rem: $\tilde{\mathbf{C}}$ is not coercive $\rightarrow$ $\mathbf{P}$ provides the "hypocoercivity norm."

In Euclidean matrix norm:

$$\left\|e^{-\tilde{\mathbf{C}}_{opt} t}\right\|_{\mathcal{B}(\mathbb{R}^d)} \leq \sqrt{\kappa(\mathbf{P})}\, e^{-\lambda_{opt} t}, \qquad t \geq 0,$$

$\kappa(\mathbf{P})$ ... condition number; can be chosen arbitrarily close to 1 with a "good" choice of $\tilde{\mathbf{C}}$. □

Proof-idea (cont'd)

4. decay of drift-ODE $\dot{y}(t) = -\tilde{\mathbf{C}}y(t)$ in norm $\|y\|^2_{\mathbf{P}} := \langle y, \mathbf{P}y\rangle$:

$$\frac{d}{dt}\|y(t)\|^2_{\mathbf{P}} = -\left\langle y(t), \left[\mathbf{P}\tilde{\mathbf{C}} + \tilde{\mathbf{C}}^T\mathbf{P}\right] y(t)\right\rangle = -2\lambda_{opt}\|y(t)\|^2_{\mathbf{P}}.$$

$$\Rightarrow \quad \|y(t)\|_{\mathbf{P}} = e^{-\lambda_{opt} t}\|y(0)\|_{\mathbf{P}}, \qquad t \geq 0.$$

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Remarks:

- $(\mathbf{C}_{opt}(c), \mathbf{D}_{opt}(c))$ is not unique; $\tilde{\mathbf{C}}^T_{opt}(c)$ yields an alternative.
- This optimal FP eq. has maximal *hypocoercivity index* $d-1$.

Outline:

1. Fokker-Planck equations with linear drift: propagator norm
2. construction of best (hypocoercive) Fokker-Planck equations
3. numerical illustrations
4. outlook: Fokker-Planck equations with t-dependent coefficients

Numerical illustration (1)

2D Example:

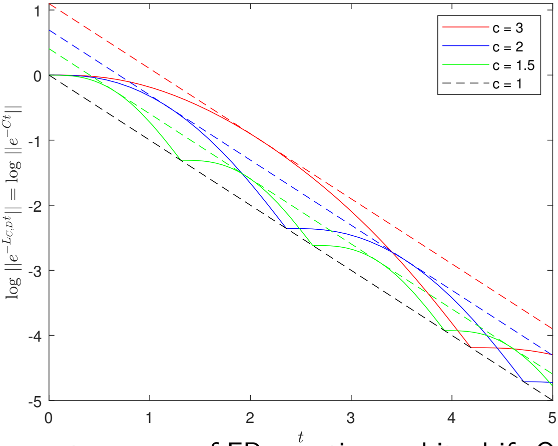
- Given covariance matrix $\mathbf{K} = \mathrm{diag}(\frac{1}{\varepsilon}, 1)$, $\varepsilon = 0.05$.
  $\Rightarrow \lambda_{opt} = \lambda_{max}(\mathbf{K}^{-1}) = 1$.
- For any $c > 1$ in the decay estimate $\|f(t) - f_{\infty,K}\|_{L^2(f_{\infty,K}^{-1})} \leq c\, e^{-\lambda_{max} t}$:

$$\Rightarrow \quad \mathbf{D}_{opt} = \tilde{\mathbf{D}}_{opt} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}$$

$$\mathbf{C}_{opt}(c) = \begin{pmatrix} 0 & -\frac{\mu}{\sqrt{\varepsilon}} \\ \sqrt{\varepsilon}\mu & 2 \end{pmatrix}, \quad \tilde{\mathbf{C}}_{opt}(c) = \begin{pmatrix} 0 & -\mu \\ \mu & 2 \end{pmatrix}, \quad \mu := \frac{c^2+1}{c^2-1}.$$

- $c \searrow 1 \Rightarrow \mu \to \infty$ ... high-rotational limit
  Practical tradeoff:
  better convergence vs. smaller matrix $\mathbf{C}$ ($\to$ allows for larger time steps in the numerics of the mentioned Markov process)

Numerical illustration of $\|f(t) - f_{\infty,K}\|_{L^2(f_{\infty,K}^{-1})} \le c\, e^{-\lambda_{max} t}$



—— exact propagator norms of FP-equation and its drift-ODE (for $c = 3$):

$$\left\| e^{-L_{C,D}t} \right\|_{\mathcal{B}(\{f_{\infty,K}\}^\perp)} = \left\| e^{-\tilde{\mathbf{C}}t} \right\|_{\mathcal{B}(\mathbb{R}^d)}, \quad t \ge 0$$

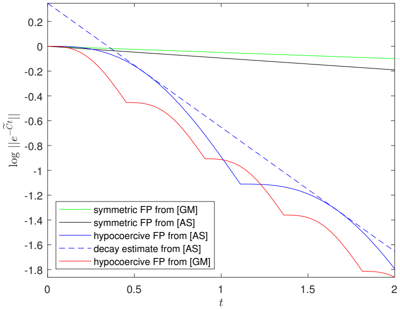
- - - corresponding exponential decay estimate (as optimal upper envelop)

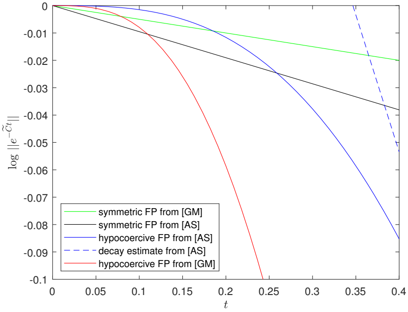
Numerical illustration: comparison to [Guillin-Monmarché]

- Given covariance matrix $\mathbf{K} = \text{diag}(\frac{1}{\varepsilon}, 1), \varepsilon = 0.05$, given $c = \sqrt{2}$.

$$\Rightarrow \quad \tilde{\mathbf{D}}_{opt} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}, \quad \tilde{\mathbf{C}}^{AS}_{opt} = \begin{pmatrix} 0 & -3 \\ 3 & 2 \end{pmatrix}, \quad \tilde{\mathbf{C}}^{GM}_{opt} = \begin{pmatrix} 0 & -7 \\ 7 & 2 \end{pmatrix}$$

- Estimate in [GM] is not sharp → more rotation than "necessary" for the bound $c\, e^{-\lambda_{max} t}$ (- - -) is used → unfavorable for time step restriction.





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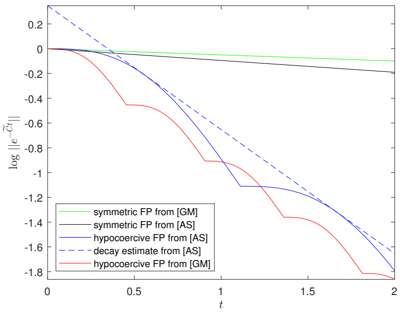

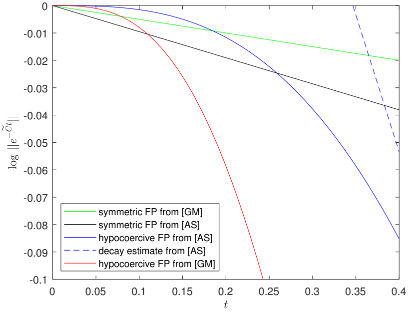

- zoom (at $t \approx 0$) on right: symmetric FP-evolution decays initially faster!

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FP with t-dependent coefficients; K ... t-independent

Let steady state $f_{\infty,K}(x) = \frac{\det(\mathbf{K})^{-1/2}}{(2\pi)^{-d/2}} \exp\left(-\frac{x^T\mathbf{K}^{-1}x}{2}\right)$, $\mathbf{K} > 0$ be given.

$$f_t = \mathrm{div}(\mathbf{D}(t)\nabla f + \mathbf{C}(t)xf), \quad (\mathbf{C}(t), \mathbf{D}(t)) \in \mathcal{I}(\mathbf{K}) \ \forall t \geq 0.$$

corresponding drift-ODE: $\frac{d}{dt}y(t) = -\tilde{\mathbf{C}}(t)y(t), \quad \tilde{\mathbf{C}}(t) := \mathbf{K}^{-\frac{1}{2}}\mathbf{C}(t)\mathbf{K}^{\frac{1}{2}}$

• A split FP-evolution yielded in [Guillin-Monmarché] a significant improvement of the decay estimate, and enabled $\|\mathbf{C}_{opt}\|_{\mathcal{F}} = \mathcal{O}(d^2)$:

$$\begin{cases} f_t = \mathrm{div}(\nabla f + \mathbf{K}^{-1}xf), & 0 \leq t \leq t_0\,, \quad \text{symmetric FP,} \\ f_t = \mathrm{div}(\mathbf{D}_{opt}\nabla f + \mathbf{C}_{opt}xf), & t > t_0\,, \quad \text{non-symm. FP.} \end{cases}$$

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• Q5: Does the symmetric FP-evolution on $[0, t_0]$ give a *true* improvement for the FP-propagator norm or 'only' a better analytic estimate?

This was difficult to decide for the PDE so far.

FP with t-dependent coefficients

Main tool:

Theorem 6 (AA-Signorello 2021)

Let $\mathbf{K} > 0$, $(\mathbf{C}(t), \mathbf{D}(t)) \in \mathcal{I}(\mathbf{K})$, $\mathbf{C}(t)$ *positive stable* $\forall\, t \geq 0$. *Then:*

$$\|S(t_2, t_1)\|_{\mathcal{B}(\{f_{\infty,K}\}^\perp)} = \|T(t_2, t_1)\|_{\mathcal{B}(\mathbb{R}^d)}\,, \qquad \forall\, 0 \leq t_1 \leq t_2 < \infty$$

- FP-propagator $S(t_2, t_1)$ maps $f(t_1) \in L^2(f_{\infty,K}^{-1})$ to $f(t_2)$.
- propagator of drift-ODE $\dot{y} = -\tilde{\mathbf{C}}(t)y$: $T(t_2, t_1)$ maps $y(t_1) \in \mathbb{R}^d$ to $y(t_2)$.

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Proof-idea:

- All FP-equations with frozen t have the same steady state $f_{\infty,K}(x)$.
- $\Rightarrow$ The FP-normalizations, the space $L^2(f_{\infty,K}^{-1})$, and the subspace decomposition $\mathcal{H} := L^2(g_\infty^{-1}) = \bigoplus_{m\in\mathbb{N}_0}^{\perp} V^{(m)}$ are all t-independent.

FP with t-dependent coefficients: 2D numerical case study

Remark on Q5: $\left\| e^{-\tilde{\mathbf{C}} t} \right\|_{\mathcal{B}(\mathbb{R}^d)} = 1 - \lambda_{min}(\tilde{\mathbf{C}}_s)\, t + \mathcal{O}(t^2) \quad \text{as } t \to 0$

$\Rightarrow$ An initially symmetric FP-evolution always decays faster than a hypocoercive FP-evolution ($\tilde{\mathbf{C}}_s = \tilde{\mathbf{D}}$; typically $\text{rank}(\tilde{\mathbf{D}}) = 1$).

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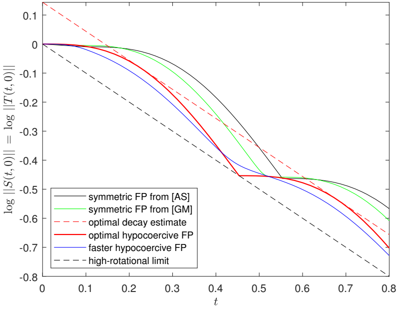
But it backfires later! Even when switching to opt. non-symmetric FP later.

- Given covariance matrix $\mathbf{K} = \text{diag}(\frac{1}{\varepsilon}, 1), \varepsilon = 0.05$, given $c := \sqrt{4/3}$.



ref. case: $\tilde{\mathbf{C}}_1 = [0\ -7; 7\ 2]\ \forall\, t \geq 0$.

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symm. FP on $t \in [0, 0.1]$, then $\tilde{\mathbf{C}}_1$.

faster rot. with $\tilde{\mathbf{C}}_2 = [0\ -11; 11\ 2]$ on $t \in [0, 0.1]$, $\tilde{\mathbf{C}}_1$ for $t \geq 0.1$ reduces const. c!

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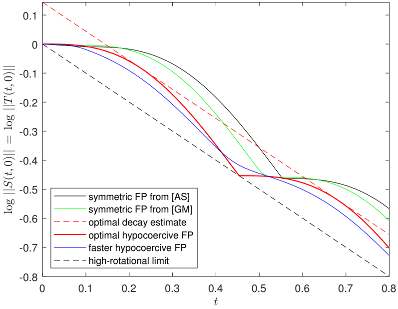

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- Open question: What is the best $\mathbf{C}(t)$, $\mathbf{D}(t)$?

Conclusion

- Construction of Fokker-Planck equations $f_t = \operatorname{div}(\mathbf{D}\nabla f + \mathbf{C}xf)$ with optimal decay.
- main tool: Propagator norms of FP-equation and corresponding drift-ODE ($\dot{x} = -\tilde{\mathbf{C}}x$) coincide.
- t-dependent coefficients can enhance the decay of Fokker-Planck equations.

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References

- A. Arnold, C. Schmeiser, B. Signorello: Propagator norm and sharp decay estimates for Fokker-Planck equations with linear drift, Comm. Math. Sci. 2022.
- A. Arnold, B. Signorello: Optimal non-symmetric Fokker-Planck equation for the convergence to a given equilibrium, KRM 2022.

Thanks for

your attention