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

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Topic & goals

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

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

  $\rightarrow$ 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 $V(x) = \frac{x^T K^{-1} x}{2}$, $K > 0$, $f_\infty(x) = c_K e^{-V(x)}$ ... anisotropic Gaussian

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Theme:

- Non-symmetric perturbations (that preserve f_∞) can enhance the convergence.
- Goal: Find optimal perturbation that yields best exponential estimate
  $$\|f(t) - f_\infty\|_{L^2(f_\infty^{-1})} \leq c\, e^{-\lambda t} \|f_0 - f_\infty\|_{L^2(f_\infty^{-1})}, \quad t \geq 0,$$
  with (1) maximal $\lambda > 0$ and (2) minimal $c \geq 1$.

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.

Outline:

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

Fokker-Planck equations with linear drift

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

$$\text{Find} \qquad f_t = \operatorname{div}(D\nabla F + Cxf) =: -L_{C,D} f \qquad \text{with fastest decay}; \qquad (1)$$

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

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

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

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Lemma 1 (Guillin-Monmarché 2016)

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

Lemma 2

Let $K > 0$, $(C,D) \in \mathcal{I}(K)$, C positive stable.
Then $f_{\infty,K}$ is the unique (normalized) steady state; (1) is hypocoercive.

Questions

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

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 (2)?
3. For a fixed $K > 0$ and the corresponding λ_{opt}, and for any $c > c_{inf}$, which pair(s) of matrices $(C_{opt}(c), D_{opt}(c) \ge 0)$ yields the convergence estimate (2) with the constants (λ_{opt}, c)?
4. For such an optimal pair of matrices, what bound on $\|C_{opt}\|$ can be found, and how does this bound grow w.r.t. to the space dimension d?

Results from the literature

Lemma 3 (Guillin-Monmarché 2016)

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

$\kappa(K)$ ... condition number

Strategy for improvement

nonsymmetric FP-equation: $f_t = \mathrm{div}(D\nabla F + Cxf) =: -L_{C,D} f$

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

Main tool:

Theorem 1 (AA-Schmeiser-Signorello 2020)

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

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

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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 2 (AA-Signorello 2021)

Let $K > 0$ be given. Then:

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

$$\left|\left|e^{-L_{C_{opt},D_{opt}}t}\right|\right|_{\mathcal{B}(V_0^\perp)} \le c\, e^{-\max(\sigma(K^{-1}))t}, \qquad t \ge 0. \tag{3}$$

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

$$||C_{opt}||_{\mathcal{F}} \le \lambda_{opt}\left[d + \sqrt{\kappa(K)}\,\frac{2\pi c^2}{\sqrt{3}(c^2-1)}\,\sqrt{d}\,(d-1)\right], \quad ||D_{opt}||_{\mathcal{F}} = d. \tag{4}$$

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

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

1. normalize FP-equation: $y := K^{-1/2}x$, $g(y) := \sqrt{\det(K)}\, f(K^{1/2}y)$

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

with $\widetilde{D} := K^{-1/2}DK^{-1/2} \geq 0$, $\widetilde{J} := K^{-1/2}JK^{-1/2} = -\widetilde{J}^T$,
$\widetilde{C} := K^{-1/2}CK^{1/2} = \widetilde{D} + \widetilde{J}$.

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

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

3. algorithmic <u>construction of $\widetilde{J}$, $P > 0$</u> such that:

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

Proof-idea (cont'd)

4. decay of drift-ODE $\dot{y}(t) = -\widetilde{C}y(t)$ in norm $\|y\|_P^2 := \langle y, Py \rangle$:

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

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

in Euclidean matrix norm:

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

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

Remark: $(C_{opt}(c), D_{opt}(c))$ is not unique; $\widetilde{C}_{opt}^T(c)$ yields an alternative.

Numerical illustration (1)

2D Example:

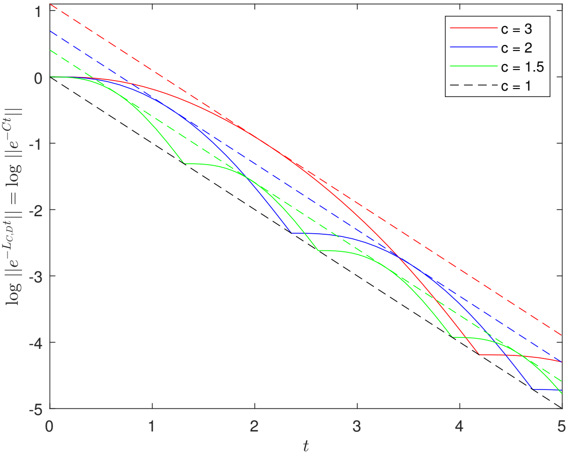
- Given covariance matrix $K = \mathrm{diag}(\frac{1}{\varepsilon}, 1)$, $\varepsilon = 0.05$.
  $\Rightarrow \lambda_{opt} = \lambda_{max}(K^{-1}) = 1$.
- Given $c > 1$ for decay estimate $\|f(t) - f_{\infty,K}\|_{L^2(f_{\infty,K}^{-1})} \le c\, e^{-\lambda_{max} t}$.

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

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

- $c \searrow 1 \Rightarrow \mu \to \infty$ ... high-rotational limit
  Tradeoff:
  better convergence vs. smaller matrix C ($\rightarrow$ larger time step size)

Numerical illustration (2)



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

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

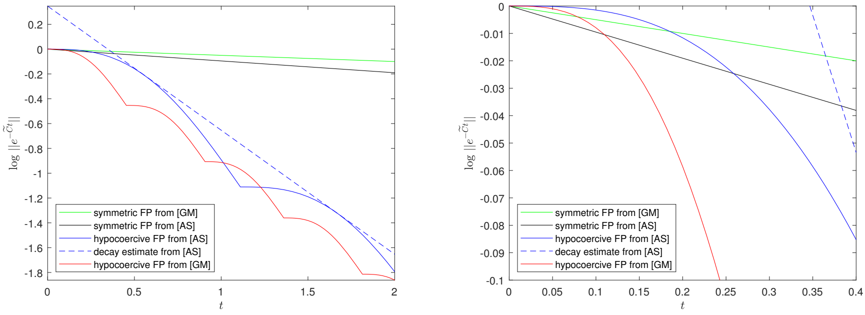
- - - corresponding exponential decay estimate (as optimal envelop above)

Numerical illustration: comparison to [Guillin-Monmarché]

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

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

- Estimate in [GM] is not sharp → more rotation than "necessary" is used → unfavorable for time step restriction.



- zoom on right: symmetric FP-evolution decays initially faster!

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

$$f_t = \operatorname{div}(D(t)\nabla F + C(t)xf), \quad \frac{d}{dt}x(t) = -\widetilde{C}(t)x(t), \quad \widetilde{C}(t) := K^{-\frac{1}{2}}C(t)K^{\frac{1}{2}}$$

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

$$\begin{cases} f_t = \operatorname{div}(\nabla f + K^{-1}xf), & 0 \le t \le t_0\,, \quad \text{symmetric FP,} \\ f_t = \operatorname{div}(D_{opt}\nabla f + C_{opt}xf), & t > t_0\,, \quad \text{non-symm. FP.} \end{cases}$$

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• Q5: Does the symmetric FP-evolution on $[0, t_0]$ give a *true* improvement for the FP-propagator norm? Difficult to decide for the PDE so far.

Main tool:

Theorem 3 (AA-Signorello 2021)

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

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

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

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

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

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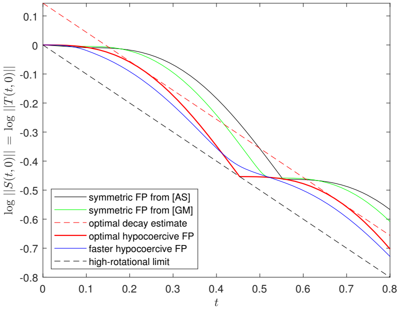
But it backfires later! Even when switching to non-symmetric FP later.

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



split FP-evolution,
on $t \in [0, 0.1]$, $t \in [0.1, \infty)$:

ref. case: $\widetilde{C}_1 = [0\ -7; 7\ 2]$, $t \geq 0$
faster rot.: $\widetilde{C}_2 = [0\ -11; 11\ 2]$
only on $[0, 0.1]$ reduces const. c

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

Conclusion

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

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- main tool: Propagator norms of FP-equation and corresponding drift-ODE ($\dot{x} = -\widetilde{C}x$) coincide.
- t-dependent coefficients can enhance the decay of Fokker-Planck equations.

References

- A. Arnold, B. Signorello: Optimal non-symmetric Fokker-Planck equation for the convergence to a given equilibrium, arXiv 2021.
- A. Arnold, C. Schmeiser, B. Signorello: Propagator norm and sharp decay estimates for Fokker-Planck equations with linear drift, arXiv 2020.