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

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

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

→ Decay estimate to $f_\infty(x) = c_\mathcal{V} e^{-V(x)}$ with rate $\inf_x \lambda_{\text{min}}(\frac{\partial^2 V}{\partial x^2})$ 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
**Topic & goals**

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

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**Theme:**

- Non-symmetric perturbations of the drift (that preserve $f_\infty$) 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)
  - needs to construct an ergodic Markov process with fast convergence to the unique measure $\mu_V$.

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

\[ f_t = \text{div} \left( D \nabla f + C x f \right) =: -Lf, \quad x \in \mathbb{R}^d \quad (1) \]

with degenerate \( 0 \leq D = D^T \in \mathbb{R}^{d \times d} \) is degenerate parabolic; (symmetric part of) \( L \) is not coercive.
degenerate Fokker-Planck equations with linear drift

\[ f_t = \text{div} \left( D \nabla f + C x f \right) =: -Lf, \quad x \in \mathbb{R}^d \]  \tag{1}

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

**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 \( \exists \lambda > 0, \ c \geq 1 \):

\[ \| e^{-Lt} f_0 \|_{\tilde{H}} \leq c \ e^{-\lambda t} \| f_0 \|_{\tilde{H}} \quad \forall \ f_0 \in \tilde{H} \]

- typically \( c > 1 \)
hypocoercive Fokker-Planck equation

\[
f_t = \text{div} \left( \mathbf{D} \nabla f + \mathbf{C} \times f \right) =: -Lf, \quad x \in \mathbb{R}^d
\]  \hspace{1cm} (2)

**Condition A:**

1. No (nontrivial) subspace of \( \text{ker} \mathbf{D} \) is invariant under \( \mathbf{C}^T \). (equivalent: \( L \) is hypoelliptic.)

2. Let \( \mathbf{C} \in \mathbb{R}^{d \times d} \) be positive stable (i.e. \( \Re(\lambda \mathbf{C}) > 0 \)).
   \[ \Rightarrow \exists \text{ confinement potential; drift towards } x = 0. \]

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

\[ \text{Lemma 1} \] Let **Condition A** hold. Then:

(2) is hypocoercive.

\[ f_\infty(x) = c K \exp \left( -x^T K^{-1} x \right) \] is the unique steady state, with \( K = K^T > 0 \) solves

\[ 2 \mathbf{D} = \mathbf{C} K + K \mathbf{C}^T \] (contin. Lyapunov eq. for \( K \))
hypocoercive Fokker-Planck equation

\[ f_t = \text{div} \left( D \nabla f + C \times f \right) = -L f, \quad x \in \mathbb{R}^d \]  

(2)

**Condition A:**

1. No (nontrivial) subspace of ker \( D \) is invariant under \( C^T \).
   (equivalent: \( L \) is hypoelliptic.)

2. Let \( C \in \mathbb{R}^{d \times d} \) be positive stable (i.e. \( \Re(\lambda^C) > 0 \)).
   \[ \Rightarrow \exists \text{ confinement potential; drift towards } x = 0. \]

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

**Lemma 1**

Let Condition A hold. Then:

1. (2) is hypocoercive.

2. \( f_\infty(x) = c_K \exp \left( -\frac{x^T K^{-1} x}{2} \right) \) is the unique steady state, with \( K = K^T > 0 \) solves \( 2D = CK + KC^T \) (continu. Lyapunov eq. for \( K \)).
normalization of Fokker-Planck equations

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

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

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

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

with \( \tilde{D} = K^{-1/2}DK^{-1/2} \Rightarrow \tilde{D} = \tilde{C}_s \geq 0 \)

Then \( g_\infty(x) = (2\pi)^{-d/2} e^{-|y|^2/2} \).
normalization of Fokker-Planck equations

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

coordinate transformation: \[ y := K^{-1/2}x, \quad g(y) := \sqrt{\det(K)} f(K^{1/2} y) \Rightarrow \]

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

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

with \[ \tilde{D} = K^{-1/2} D K^{-1/2} \Rightarrow \tilde{D} = \tilde{C}_s \geq 0 \]

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

\[ L^2 \text{-propagator norm (} \rightarrow \text{ our main tool):} \]

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

Let Condition A hold. Then:

\[ \left\| e^{-Lt} \right\|_{\mathcal{B}(\{f_\infty\}^\perp)} = \left\| e^{-\tilde{L}t} \right\|_{\mathcal{B}(\{g_\infty\}^\perp)} = \left\| e^{-\tilde{C}t} \right\|_{\mathcal{B}(\mathbb{R}^d)}, \quad \forall t \geq 0 \]
$L^2$–propagator norm

propagator norm of Fokker-Planck equ. in 2D: $\|e^{-Lt} - \Pi_0\|_{B(L^2(f^{-1}_\infty))}$
Proof of Theorem 2; for normalized FP (step 1)

Theorem 3

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

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

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

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

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

$$\sigma(L) = \left\{ \sum_{j=1}^{d} \alpha_j \lambda_j, \ \alpha \in \mathbb{N}_0^d \right\}; \quad \lambda_j \ldots \text{eigenvalues of } \tilde{C} \in \mathbb{R}^{d \times d}$$
Proof (step 2): evolution in subspaces \( V^{(m)} \)

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

ex. \( d = 2 \):

- \( m = 1 \): \( \frac{d}{dt} d_{(1,0)}^{(d_{(1,0)})} = -\tilde{C} d_{(1,0)}^{(d_{(1,0)})} \) ... drift-ODE
Proof (step 2): evolution in subspaces $V^{(m)}$

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

ex. $d = 2$:

- $m = 1$: \[ \frac{d}{dt} \begin{pmatrix} d_{(1,0)}^{(1,0)} \\ d_{(0,1)}^{(1,0)} \end{pmatrix} = -\tilde{\mathbf{C}} \begin{pmatrix} d_{(1,0)}^{(1,0)} \\ d_{(0,1)}^{(1,0)} \end{pmatrix} \] ... drift-ODE

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

better: $D^{(2)}(t) := \begin{pmatrix} d_{(2,0)} & d_{(1,1)}/2 \\ d_{(1,1)}/2 & d_{(0,2)} \end{pmatrix}(t) \in \mathbb{R}^{2\times2}$

\[ \frac{d}{dt} D^{(2)} = - \left( \tilde{\mathbf{C}} D^{(2)} + D^{(2)} \tilde{\mathbf{C}}^T \right) \]
Proof (step 2): evolution in subspaces $V^{(m)}$

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

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\[ \frac{d}{dt} D^{(2)} = - (\tilde{\mathcal{C}} D^{(2)} + D^{(2)} \tilde{\mathcal{C}}^T) \]

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

\[ \frac{d}{dt} D^{(m)}(t) = - m \text{ Sym} \left( \tilde{\mathcal{C} \circ D^{(m)}(t)} \right) \] ... tensored drift-ODE

mult. on 1st index
Proof (step 2): evolution in subspaces $V^{(m)}$

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

ex. $d = 2$:

- $m = 1$: $\frac{d}{dt}(d_{(1,0)}^{(1,0)}) = -\tilde{C}(d_{(0,1)}^{(1,0)})$ ... drift-ODE

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

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

\[
\frac{d}{dt} D^{(2)} = - (\tilde{C} D^{(2)} + D^{(2)} \tilde{C}^T)
\]

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

\[
\frac{d}{dt} D^{(m)}(t) = -m \text{ Sym} \left( \tilde{C} \odot D^{(m)}(t) \right) \quad \text{... tensored drift-ODE}
\]

\[
\text{mult. on 1st index}
\]

$\Rightarrow$ 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:

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

  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

\[ D^{(m)}(t) = \sum_{k=1}^{s} \mu_k [v_k(t)]^{\otimes m}, \quad \dot{v}_k = -\tilde{C} v_k. \]
Proof (step 3): evolution in subspaces $V^{(m)}$

- practical ingredient for estimating the evolution equation in $V^{(m)}$:
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$$D^{(m)}(t) = \sum_{k=1}^{s} \mu_k [v_k(t)]^\otimes m, \quad \dot{v}_k = -\tilde{C}v_k.$$  

- 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
  → equivalent to drift-ODE: $\| e^{-\tilde{\mathcal{C}}t} \|_2$
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3. numerical illustrations
4. outlook: Fokker-Planck equations with $t$-dependent coefficients
(non-normalized) 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.

Find \( f_t = \text{div}(D \nabla f + C x f) =: -L_{C,D} f \) with fastest decay; (4)

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

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

- Without constraint \( \text{Tr}(D) \leq d \) arbitrary decay possible \( \rightarrow \) ill-posed.
(non-normalized) 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.

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

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

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

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

Lemma 3 (Guillin-Monmarché 2016)

\[
\mathcal{I}(K) = \{D \geq 0, \text{Tr}(D) \leq d; \ C = (D + J)K^{-1}, J^T = -J\}.
\]

Lemma 4

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

hypocoercivity: \[ \| f(t) - f_{\infty},K \|_{L^2(f_{\infty}^{-1},K)} \leq c e^{-\lambda t} \| f_0 - f_{\infty},K \|_{L^2(f_{\infty}^{-1},K)}, \quad t \geq 0 \] (5)

Q1 Which FP-evolutions converge the fastest, i.e. with largest rate \( \lambda_{opt} \) to the steady state in the operator norm of \( e^{-L_c,D^t} \) on \( \{f_{\infty},K\}^\perp \subset \mathcal{H} := L^2(\mathbb{R}^d, f_{\infty}^{-1},K) \)?

Q2 When the best decay rate is fixed, what is the infimum of the multiplicative constant, \( c_{inf} \), in the decay estimate (5)?

Q3 For a fixed \( K > 0 \) and the corresponding \( \lambda_{opt} \), and for any \( c > c_{inf} \), which pair(s) of matrices \( (C_{opt}(c), D_{opt}(c) \geq 0) \) yields the convergence estimate (5) with the constants \( (\lambda_{opt}, c) \)?

Q4 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 5 (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 $\|C_{opt}\| = O(d^2)$ (with piecewise constant coefficients).

$\kappa(K)$ ... condition number
Strategy for improvement

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

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:

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

non-symmetric FP-equation:
\[ f_t = \text{div}(D \nabla f + Cf) =: -L_{C,D}f \]
corresponding drift-ODE:
\[ \frac{d}{dt} y(t) = -\tilde{C}y(t), \quad \tilde{C} := K^{-1/2}CK^{1/2} \]

Main tool:

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

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

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

- 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 $K > 0$ be given. Then:

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

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

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

$$\left\| C_{opt} \right\|_F \leq \lambda_{opt} \left[ d + \sqrt{\kappa(K)} \frac{2\pi c^2}{\sqrt{3(c^2 - 1)}} \sqrt{d(d-1)} \right], \quad \left\| D_{opt} \right\|_F = d. \quad (7)$$

$\|C\|_F$ ... Frobenius norm
Proof-idea (refinement of [Lelièvre-Nier-Pavliotis 2013], [Guillin-Monmarché 2016])

1. Normalize FP-equation: \( y := K^{-1/2} x \)

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

with \( \tilde{D} := K^{-1/2} DK^{-1/2} \geq 0, \quad \tilde{J} := K^{-1/2} JK^{-1/2} = -\tilde{J}^T, \quad \tilde{C} := K^{-1/2} CK^{1/2} = \tilde{D} + \tilde{J}. \)
Proof-idea (refinement of [Lelièvre-Nier-Pavliotis 2013], [Guillin-Monmarché 2016])

1. Normalize FP-equation: \( y := K^{-1/2}x \)

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

2. Construction of \( D \):

Maximal decay rate of \( e^{-\tilde{C}t}, \lambda_{opt} = \lambda_{max}(K^{-1}) \) only possible if \( \text{ran}(D) \subset \text{eigenspace}_{\lambda_{max}}(K^{-1}) \);

e.g. \( D := d \ v \otimes v \) (with \( K^{-1}v = \lambda_{opt}v, \|v\| = 1 \)) ... rank 1.
Proof-idea (refinement of [Lelièvre-Nier-Pavliotis 2013], [Guillin-Monmarché 2016])

1. Normalize FP-equation: \( y := K^{-1/2}x \)

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

   with \( \tilde{D} := K^{-1/2}DK^{-1/2} \geq 0, \tilde{J} := K^{-1/2}JK^{-1/2} = -\tilde{J}^T, \)

   \( \tilde{C} := K^{-1/2}CK^{1/2} = \tilde{D} + \tilde{J}. \)

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

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

   \[
   P \begin{pmatrix} \tilde{D} + \tilde{J} \\ \tilde{D} - \tilde{J} \end{pmatrix} = \begin{pmatrix} \tilde{C} \\ \tilde{C}^T \end{pmatrix} = 2\lambda_{opt}P \quad \text{... continuous Lyapunov equation for } P
   \]
Proof-idea (cont’d)

\[ \dot{y}(t) = -\tilde{C}y(t) \text{ in norm } \|y\|_P^2 := \langle y, Py \rangle: \]

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

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

Rem: \( \tilde{C} \) is not coercive \( \rightarrow \) \( P \) provides the “hypocoercivity norm.”

In Euclidean matrix norm:

\[ \|e^{-\tilde{C}_{opt} t}\|_{B(\mathbb{R}^d)} \leq \sqrt{\kappa(P)} e^{-\lambda_{opt} t}, \quad t \geq 0, \]

\( \kappa(P) \) ... condition number; can be chosen arbitrarily close to 1 with a “good” choice of \( \tilde{C} \).
Proof-idea (cont’d)

\[ \text{decay of drift-ODE } \dot{y}(t) = -\tilde{C}y(t) \text{ in norm } \|y\|_{P}^{2} := \langle y, Py \rangle : \]

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

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

Rem: \( \tilde{C} \) is not coercive \( \rightarrow P \) provides the “hypocoercivity norm.”

In Euclidean matrix norm:

\[ \|e^{-\tilde{C}_{opt}t}\|_{B(\mathbb{R}^d)} \leq \sqrt{\kappa(P)} e^{-\lambda_{opt}t}, \quad t \geq 0, \]

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

Remarks:

• \( (C_{opt}(c), D_{opt}(c)) \) is not unique; \( \tilde{C}_{opt}^{T}(c) \) 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 $\mathbf{K} = \text{diag}(1/\varepsilon, 1), \varepsilon = 0.05.$
  $\Rightarrow \lambda_{opt} = \lambda_{\text{max}}(\mathbf{K}^{-1}) = 1.$

- For any $c > 1$ in the decay estimate $\|f(t) - f_{\infty, \mathbf{K}}\|_{L^2(f_{\infty, \mathbf{K}}^{-1})} \leq c e^{-\lambda_{\text{max}} t}:

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

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

- $c \downarrow 1 \Rightarrow \mu \to \infty$ ... 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 $\|f(t) - f_{\infty,K}\|_{L^2(f_{\infty,K}^{-1})} \leq c e^{-\lambda_{\text{max}} t}$

- exact propagator norms of FP-equation and its drift-ODE (for $c = 3$):  
  \[ \left\| e^{-L_{c,D}t} \right\|_{B(\{f_{\infty,K}\}^\perp)} = \left\| e^{-\tilde{c}t} \right\|_{B(\mathbb{R}^d)}, \quad t \geq 0 \]

- corresponding exponential decay estimate (as optimal upper envelop)
Numerical illustration: comparison to [Guillin-Monmarché]

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

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

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

\begin{itemize}
  \item zoom (at $t \approx 0$) on right: symmetric FP-evolution decays initially faster!
\end{itemize}
Numerical illustration: comparison to [Guillin-Monmarché]

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

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1. Fokker-Planck equations with linear drift: propagator norm
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FP with $t$-dependent coefficients; $K$ ... $t$-independent

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.

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

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

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

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

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  f_t = \text{div}(D_{opt} \nabla f + C_{opt} xf), & t > t_0, \quad \text{non-symm. FP}.
\end{cases}
\]

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

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

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

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- FP-propagator $S(t_2, t_1)$ maps $f(t_1) \in L^2(f_{\infty,K}^{-1})$ to $f(t_2)$.
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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 $\mathcal{H} := L^2(g_{\infty,K}^{-1}) = \bigoplus_{m \in \mathbb{N}_0} V(m)^\perp$ are all $t$-independent.
FP with $t$-dependent coefficients: 2D numerical case study

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

\[\Rightarrow\] An initially symmetric FP-evolution always decays faster than a hypocoercive FP-evolution ($\tilde{C}_s = \tilde{D}$; typically rank($\tilde{D}$) = 1).
FP with $t$-dependent coefficients: 2D numerical case study

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

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

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

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

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

split FP-evolutions:
- symm. FP on $t \in [0, 0.1]$, then $\tilde{C}_1$.
- faster rot. with $\tilde{C}_2 = [0 \ -11; 11 \ 2]$ on $t \in [0, 0.1]$, $\tilde{C}_1$ for $t \geq 0.1$

reduces const. $c$!
Remark on Q5: \( \| e^{-\tilde{C} t} \|_{B(\mathbb{R}^d)} = 1 - \lambda_{\min}(\tilde{C}_s) t + O(t^2) \) as \( t \to 0 \)

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

But it backfires later! Even when switching to opt. non-symmetric FP later.
• Given covariance matrix \( K = \text{diag}(\frac{1}{\varepsilon}, 1) \), \( \varepsilon = 0.05 \), given \( c := \sqrt{4/3} \).

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

split FP-evolutions:
symm. FP on \( t \in [0, 0.1] \), then \( \tilde{C}_1 \).

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

• Open question: What is the best \( C(t), D(t) \) ?
Conclusion

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

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

References

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Thanks for your attention