On ensemble optimal control problems governed by Liouville, Fokker-Planck and linear Boltzmann equations

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Before starting....

Announcements and acknowledgements
Modelling with ODE

Ordinary Differential Equations

A Comprehensive Approach

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BMBF joint project on MR Imaging and Deep Learning

Intelligent MR Diagnosis of the Liver by Linking Model and Data-driven Processes (iDeLIVER)

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Dynamical models

Many dynamical models of interest in sciences belong to one of these classes

1. Deterministic models:
   \[ \dot{X}(t) = a(X(t), t) \]

2. Stochastic drift-diffusion-jump models:
   \[ dX(t) = a(X(t), t) \, dt + \sigma \, dW(t) + dP(t) \]

3. Piecewise-deterministic processes:
   \[ \dot{X}(t) = a_{S(t)}(X(t), t), \quad t \in [0, \infty) \]

where \( a = a(x, t) \) is called the drift, \( \sigma \) is the dispersion coefficient, \( W(t) \) is the Wiener process, \( P(t) \) is a compound Poisson process, \( S(t) : [0, \infty) \to S \) is a Markov process with a discrete set of states, \( S = \{1, \ldots, S\} \).

Many evolution PDEs represent the emergent equations from the microscopic underpinnings of the models above (J. Hopfield).

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Left: Trajectories of a **drift-diffusion-jump** model: \( a(x, t) = -4 \, x \), \( \sigma = 2 \), and initial condition \( X(0) = 0 \).

Right: Trajectories of a **PDP process**: \( a_1(x, t) = -4 \, x + 2 \), \( a_2(x, t) = -4 \, x - 2 \), and initial condition for both states \( X(0) = 0 \).

In general, the initial condition \( X(0) = X_0 \) is given by means of a distribution function \( f_0(x) \). In this case, also the **deterministic model** results in an ensemble of trajectories.
Density functions

It appears that one can identify different realisations (trajectories) of a single dynamical system with the trajectory of multiple copies of the same (non-interacting) system.

In both pictures, consideration of all trajectories separately is an overwhelming task. For this reason, Ludwig Eduard Boltzmann introduced the concept of (material) density of the configuration (position, velocity, etc.) of the system.

In particular, if \( f_0(x) \) represents the spatial density of non-interacting particles at time \( t = 0 \) and subject to a (divergence free) velocity field \( a(x, t) \), then the evolution of this density is modelled by the Liouville equation\(^1\):

\[
\frac{\partial}{\partial t} f(x, t) + \text{div} \left( a(x, t) f(x, t) \right) = 0,
\]

with initial condition \( f(x, 0) = f_0(x) \).

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\(^1\) L. Boltzmann, ‘Vorlesungen über Gastheorie’ (1896-1898)
Liouville equation

\[ \partial_t f(x, t) + \text{div} \left( a(x, t) f(x, t) \right) = 0, \quad f(x, 0) = f_0(x). \]

With appropriate \( a \) and smooth \( f_0 \), we can obtain \( f \) by the formula

\[ f(x, t) = \frac{1}{\det J(t, \psi_t^{-1}(x))} f_0(\psi_t^{-1}(x)), \]

where \( \psi_t(x) = \psi(t, x) \) denotes the flow map associated to \( a \), \( J(t, x) = \nabla_x \psi_t(x) \) is its Jacobian matrix, and \( \psi_t^{-1}(x) \) means the inverse with respect to the space variable, at \( t \) fixed. By definition of flow map, \( \psi \) verifies the equation

\[ \partial_t \psi(t, x) = a(\psi(t, x), t), \quad \psi(0, x) = x. \]
Consider a continuous-time continuous-space stochastic process with $X : \mathcal{I} \times \Omega \rightarrow \mathbb{R}$, and $\text{Range}(X) = \mathbb{R}$. Since different random variables are labelled by different $t$ in $\mathcal{I} = [0, +\infty)$, we can denote the probability density function (PDF) of the random variable $X$ at $t \in \mathcal{I}$ with $f(\cdot, t)$.

Similarly, we denote with $f(\cdot, t_2 \mid v_1, t_1)$ the conditional probability (transition) density function of $X(t_2, \omega)$ given the occurrence of the value $v_1$ of $X(t_1, \omega)$ with $f(v_1, t_1) > 0$.

For a Markov process, we have $f(v, t) = \int_{\mathbb{R}} f(v, t \mid z, 0) f_0(z) \, dz$, and continuity implies the following identity

$$f(v, \tau \mid z, t) = \int_{\mathbb{R}} f(v, \tau \mid r, s) f(r, s \mid z, t) \, dr,$$

where $\tau > s > t$. This is the Chapman-Kolmogorov equation for the conditional PDFs.

Notice that, in this probabilistic framework, we have $\int_{\mathbb{R}} f_0(x) \, dx = 1$, and so $\int_{\mathbb{R}} f(x, t) \, dx = 1$, $t \geq 0$. 
Einstein, Fokker-Planck, Kolmogorov, ... equations

With the Chapman-Kolmogorov equation and specification of the probability space \((\Omega, \mathcal{F}, P)\) for the random variable \(X(t, \cdot)\) with \(t\) fixed, one can (re-)obtain the evolution equations for the PDF.

For the deterministic case, we have the Liouville equation.

For the stochastic drift-diffusion-jump process, we have

\[
\partial_t f(x, t) + \partial_x (a(x, t) f(x, t)) = \frac{\sigma^2}{2} \partial_{xx} f(x, t) + \lambda \int_{\mathbb{R}} [f(x - y, t) - f(x, t)] g(y) \, dy.
\]

where \(P_t\) is exp distributed in time with \(\lambda e^{-\lambda \Delta t}\), \(\lambda\) the rate of jumps, whose amplitude is distributed according to \(g = g(x)\).

For the piecewise-deterministic process, we have

\[
\partial_t f_s(x, t) + \partial_x (a_s(x, t) f_s(x, t)) = \sum_{j=1}^{S} Q_{sj}(x) f_j(x, t), \quad s = 1, \ldots, S,
\]

where \(Q_{sj}\) is given by \(Q_{sj} = \begin{cases} \mu_j q_{sj} & \text{if } j \neq s, \\ \mu_s (q_{ss} - 1) & \end{cases}\)

2 corresponding to a stochastic transition probability matrix \(\{q_{ij}\}\) and switching times with exponential PDF of transition events \(\psi_s(t) = \mu_se^{-\mu_st}\).  

Continuity equations

We see that the differential form of the Chapman-Kolmogorov equation (also known as the master equation) results in different PDE models that describe continuity and conservation of the total probability of the state of a stochastic process. They all have the Liouville operator as an essential component.

On the other hand, Boltzmann derived his equation for the evolution of material density starting from the Liouville equation (theorem). He augmented this equation with a nonlinear collision term as follows $^3$.

$$\partial_t f(x, v, t) + a \cdot \nabla_x f(x, v, t) + b \cdot \nabla_v f(x, v, t) = C_u[f](x, v, t)$$

Notice that, in this case, the configuration of the system is determined by the position and velocity of the particles (phase space); $a$ denotes the velocity field and $b$ the acceleration field.

In all these continuity equations, boundary conditions result by given barrier/requirements on the (microscopic) dynamical models.

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Connections between the continuity equations

The different continuity equations are related (a few references):

- A nonlinear Boltzmann equation becomes linear for a massive particle $M$ immersed in a viscous fluid and subject to collision of much smaller particles of mass $m \ll M$ (Brownian motion)\(^4\)

- A linear Boltzmann equation becomes the drift-diffusion (Fokker-Planck) equation in the small-diffusion limit (Kramers-Moyal expansion)\(^5\)

- The Liouville equation results by vanishing viscosity of the Fokker-Planck equation\(^6\)

- The linear and nonlinear Boltzmann equations can be framed in the PDP framework\(^7\)

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Optimal control of a dynamical system

Consider the following optimal control problem of a deterministic model

$$\min J(X, u) := \int_0^T \ell(t, X(t), u(t)) \, dt + \varphi(X(T))$$

s.t. \( \dot{X}(t) = a(X(t), t; u(t)) \)

\( X(0) = X_0 \),

The dynamical model now includes a control mechanism and \( u \) denotes the control function.

Suppose that the purpose of the control is for the system to track a desired trajectory \( x_D : [0, T] \to \mathbb{R}^d \) and attain a target configuration at final time given by \( x_T \in \mathbb{R}^d \). We choose

$$\ell(t, X(t), u(t)) = \theta(X(t), t) + \kappa(u(t)),$$

where \( \theta(\cdot, t) \), \( \varphi(\cdot) \) and \( \kappa(\cdot) \) are convex functions. Usual choice:

$$\theta(x, t) = (x - x_D(t))^2, \quad \varphi(x) = (x - x_T)^2, \quad \kappa(u) = u^2.$$
Ensemble optimal control problems

An ensemble optimal control problem\(^8\) considers the minimisation of the expected value of the tracking part of the cost functional with respect to all possible trajectories of the dynamical system with initial condition specified by an initial density \( f_0 \).

\[
J(f, u) := \mathbb{E}\left[ \int_0^T \theta(t, X(t)) \, dt + \varphi(X(T)) \right] + \int_0^T \kappa(u(t)) \, dt
\]

\[
= \int_0^T \int_{\mathbb{R}^d} \theta(x, t) \, f(x, t) \, dx \, dt + \int_{\mathbb{R}^d} \varphi(x) \, f(x, T) \, dx + \int_0^T \kappa(u(t)) \, dt
\]

subject to the differential constraint given by the (controlled) Liouville equation

\[
\partial_t f(x, t) + \text{div} \left( a(x, t; u(t)) \, f(x, t) \right) = 0, \quad f(x, 0) = f_0(x).
\]

Notice that for a function \( g = g(x, t) \) we write the expected value at \( t \) as follows: \( \mathbb{E}[g](t) = \int_{\mathbb{R}^d} g(x, t) \, f(x, t) \, dx \).

Further, notice that the specification of \( \theta(\cdot, t) \), \( \varphi(\cdot) \) as convex functions is problematic.

Remarks on Brockett’s ensemble control problems

Brockett’s aim is to construct control functions $\tilde{u}(x, t)$ based on $u = u(t)$ as vector of coefficients of a polynomial of $x$. It has multiple aims:

1. **Open-loop and closed-loop strategies** can be both accounted for by considering the control function $\tilde{u}(x, t)$:
   - **Open-loop**: the functional dependence on $x$ is given while dependence on $t$ (i.e. $u = u(t)$) must be determined;
   - **Closed-loop**: the functional dependence on both $x$ and $t$ must be determined.

2. Also in the open-loop case a robust control can be obtained.

3. Appropriate choice of the functional dependence of $\tilde{u}$ on $x$ may allow to obtain a good approximation of the closed-loop control function while being easier to implement.

4. This framework can be applied for the design of control schemes for different models using the corresponding continuity equations.

Theoretical and numerical work is required for the rigorous formulation and efficient numerical solution of ensemble optimal control problems.
A Liouville ensemble optimal control problem

We focus on a 2D Liouville ensemble optimal control problem:\n
\[
\min_{u \in U_{ad}} J(f, u) := \int_0^T \int_{\mathbb{R}^2} \theta(x, t) f(x, t) \, dx \, dt + \int_{\mathbb{R}^2} \phi(x) f(x, T) \, dx + \int_0^T \kappa(u(t)) \, dt
\]

s.t. \( \partial_t f(x, t) + \text{div} \left( a(x, t; u) f(x, t) \right) = 0, \quad f(x, 0) = f_0(x). \)

The drift \( a(x, t; u) \) includes two control functions \( u_1(t), u_2(t) \in \mathbb{R}^2 \), \( u = (u_1, u_2) \), and the purpose of this control is to drive \( f \) such that the cost functional \( J \) is minimized.

In the realm of control of ODEs, one usually considers linear and bilinear control mechanisms. Thus, we choose

\[
a(x, t; u) = a_0(x, t) + bu_1(t) + c x \circ u_2(t)
\]

where \( a_0 \) is a given smooth vector field, which is Lipschitz in \( x \), and \( b, c \in \mathbb{R} \) are constants; \( x = (x_1, x_2) \).

\footnote{J. Bartsch, A. Borzì, F. Fanelli, S. Roy, A theoretical investigation of Brockett’s ensemble optimal control problems, Calculus of Variations and Partial Differential Equations (2019).}
**Attracting potentials**

We refer to $\theta$ as an attracting potential, and focus on the following choice

$$\theta(x, t) = -\alpha \exp \left( -\frac{|x - x_D(t)|^2}{2\sigma_\theta^2} \right), \quad \alpha > 0, \quad \sigma_\theta > 0.$$  

Similarly, by the requirement that the density $f$ at final time concentrates on a final position denoted with $x_T \in \mathbb{R}^d$, we have

$$\varphi(x) = -\beta \exp \left( -\frac{|x - x_T|^2}{2\sigma_\varphi^2} \right), \quad \beta > 0, \quad \sigma_\varphi > 0.$$  

**Moment equations**

In the simplest case $a(x, t; u) = u_1(t) + x \circ u_2(t)$, and assuming that $f_0$ is Gaussian, we obtain the moment equations

$$\dot{m}(t) = u_1(t) + m(t) u_2(t), \quad m(0) = x_0,$$

$$\dot{v}(t) = 2 \nu(t) u_2(t), \quad \nu(0) = \nu_0.$$  

for the mean $m(t) = \mathbb{E}[x](t)$ and the variance $\nu(t) = \mathbb{E}[(x - m(\cdot))^2](t)$.

On the other hand, the ensemble control framework allows a general form of the drift and multimodal distributions.
Control space and admissible set

We consider the following function\(^{10}\)

\[
\kappa(u(t)) := \frac{\gamma}{2} |u(t)|^2 + \delta |u(t)| + \frac{\nu}{2} \left| \frac{du}{dt}(t) \right|^2
\]

where \(\gamma, \nu > 0\) and \(\delta \geq 0\). It is clear that, with this setting, the control space \(U\) corresponds to a weighted \(H^1\) space given by \(\tilde{H}^1_T := \tilde{H}^1_T \times \tilde{H}^1_T\), where \(\tilde{H}^1_T\) corresponds to the \(H^1([0, T]; \mathbb{R}^2)\) space, endowed with the following weighted \(H^1\)-product

\[
(u, v)_{\tilde{H}^1_T} := \gamma \int_0^T u(t) \cdot v(t) \, dt + \nu \int_0^T u'(t) \cdot v'(t) \, dt.
\]

The notation \(\' = d/dt\) stands for the weak time derivative.
We have the set of admissible controls

\[
U_{ad} = \{ v \in H^1_0([0, T]; \mathbb{R}^2) \times H^1_0([0, T]; \mathbb{R}^2) : u_a \leq u(t) \leq u_b, \ t \in [0, T] \}.
\]

Existence and uniqueness of solutions for unbounded drift

\[
\partial_t f + \text{div} (a(x, t; u) f) = g, \quad f(x, 0) = f_0(x)
\]

\[
\left\{
\begin{array}{l}
g \in L^1([0, T]; H^m(\mathbb{R}^d)) \quad \text{and} \quad f_0 \in H^m(\mathbb{R}^d) \\
a \in L^1([0, T]; C^{m+1}(\mathbb{R}^d)), \quad \text{with} \quad \nabla a \in L^1([0, T]; C^m_b(\mathbb{R}^d)).
\end{array}
\right.
\]

**Theorem**

Let \( T > 0 \) and \( m \in \mathbb{N} \) fixed, and let \( a, f_0 \) and \( g \) satisfy our hypotheses. Then there exists a unique solution \( f \in C([0, T]; H^m(\mathbb{R}^d)) \) of the Liouville initial-value problem. Moreover, there exists a “universal” constant \( C > 0 \), independent of \( f_0, a, g, f \) and \( T \), such that the following holds true for any \( t \in [0, T] \):

\[
\|f(t)\|_{H^m} \leq C \left( \|f_0\|_{H^m} + \int_0^t \|g(\tau)\|_{H^m} \, d\tau \right) \exp \left( C \int_0^t \|\nabla a(\tau)\|_{C^m_b} \, d\tau \right).
\]

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Existence of solutions of the optimization problem

By introducing the control-to-state map $G$, we have the following formulation of the Liouville ensemble control problem

$$\min_{u \in U_{ad}} \hat{J}(u) := J(G(u), u),$$

**Theorem**

The Liouville ensemble optimal control problem with $\gamma > 0$, $\delta \geq 0$, $\nu \geq 0$ admits at least one solution $u^* \in U_{ad}$. The corresponding state $f^* := G(u^*)$ belongs to the space $C([0, T]; H^m_k(\mathbb{R}^d)), (m, k) \in \mathbb{N}^2$.

The mathematical formulation of the Liouville model requires the functional spaces:

For $1 \leq p < \infty$ and a Banach space $X$, we define the Bochner-spaces $L^p_T(X) := L^p([0, T]; X)$, and for $m \in \mathbb{N}_0$, $C^m_T(X) := C^m([0, T], X)$. Further, for $(m, k) \in \mathbb{N}^2$, $m \leq k$ fixed, we define the space $H^m_k(\mathbb{R}^d)$ as follows

$$H^0_k(\mathbb{R}^d) = L^2_k(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) \mid |x|^k f \in L^2(\mathbb{R}^d) \right\},$$

and, for $m \geq 1$, we set

$$H^m_k(\mathbb{R}^d) := \left\{ f \in H^m(\mathbb{R}^d) \cap H^{m-1}_k(\mathbb{R}^d) \mid |x|^k D^\alpha f \in L^2(\mathbb{R}^d) \quad \forall |\alpha| = m \right\}.$$

Notice that, for all fixed $m$ and $k$ in $\mathbb{N}$, one has the embedding $H^m_k \subset H^m$. 

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Optimality system

Since $J$ and $G$ are Fréchet differentiable, we can characterize an optimal control as the solution of the first-order optimality condition for $\min_{u \in U_{ad}} \hat{J}(u)$.

The optimality system for $\nu = 0$ is given by, with $\hat{\lambda} \in \partial \left( \delta \|u\|_{L^1_T} \right)$ and $q$ being the Lagrange multiplier,

$$\begin{align*}
\partial_t f + \text{div} \left( a(x, t; u) f \right) &= 0, \quad \text{with } \rho|_{t=0} = \rho_0 \\
- \partial_t q - a(x, t; u) \cdot \nabla q &= -\theta, \quad \text{with } q|_{t=T} = -\varphi \\
\left( \gamma u^r_j + \hat{\lambda}^r_j + \int_{\mathbb{R}^d} \text{div} \left( \frac{\partial a}{\partial u^r_j} f \right) q \, dx, \, v^r_j - u^r_j \right)_{L^2(0, T)} &\geq 0 \\
\forall v \in U_{ad}, \, j = 1, 2, \, r = 1 \ldots d
\end{align*}$$

The case $\nu > 0$ is more involved since it requires to construct the reduced gradient in the space $\tilde{H}^1_T$ and appropriate $H^1$ projection to implement the box constraints (see Bartsch et al.).
**Numerical approximation**

We develop a **cell-centred finite-volume** scheme on equally spaced, non-overlapping cells, on a sufficiently large square domain $\Omega$. \(^{14}\)

**Liouville equation**

- Implement a strong stability conserving Runge-Kutta method of second order in time and Kurganov-Tadmor\(^{15}\) scheme in space (**SSPRK2-KT**)

**Adjoint Liouville equation**

- As above and **Strang splitting** \(^{16}\)

**Optimality condition/reduced gradient**

- Rectangular quadrature, finite differences.

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\(^{14}\) J. Bartsch, A. Borzi, F. Fanelli, S. Roy, A numerical investigation of Brockett’s ensemble optimal control problems.


Properties of SSPRK2-KT

**Lemma.** The semi-discrete KT scheme is at least second order accurate for smooth $f$, except at the points of extrema of $f$.

**Lemma.** The Kurganov-Tadmor scheme is conservative, in the sense that $\sum_{i,j}^{N_x} f_{i,j}^k = \sum_{i,j}^{N_x} f_{i,j}^0$, $k = 1, \ldots, N_t$.

**Lemma.** The solution $f_{i,j}^k$ obtained with the SSPRK2-KT-scheme is discrete $L^1$ stable in the sense that

$$\|f^k\|_1 = \|f_0\|_1, \quad k = 0, \ldots, N_t - 1$$

under the CFL condition

$$\frac{\Delta t}{h} \| a_1 \|_{L^\infty_T L^\infty} = \frac{\Delta t}{h} \max_{t \in [0,T]} \max_{x \in \Omega} |a_1(x, t; u(t)| \leq \frac{1}{4},$$

$$\frac{\Delta t}{h} \| a_2 \|_{L^\infty_T L^\infty} = \frac{\Delta t}{h} \max_{t \in [0,T]} \max_{x \in \Omega} |a_2(x, t; u(t)| \leq \frac{1}{4}.$$
Accuracy results

Theorem

The solution $f_h$ of the SSPRK2-KT scheme is second-order accurate in the $L^1$-norm as follows

$$\| f_h(\cdot, T) - f(\cdot, T) \|_1 \leq c(T) h^2,$$

except at the point of extrema of the exact solution $f$ of the Liouville equation.

Theorem

Let $q(x, t)$ be the solution of the Liouville adjoint equation and $q_h(x, t)$ be the corresponding numerical solution using the Strang-SSPRK2-KT scheme. Then under the CFL-condition the following error estimates holds except at points of extrema of $q$

$$\| q_h(\cdot, 0) - q(\cdot, 0) \|_1 \leq \tilde{c}(T) h^2,$$

where $\tilde{c}$ does not depend on $h$ or $\Delta t$. 
Optimization algorithm

**Algorithm 1** Semi-smooth Newton method

**Require:** $u_0, f_0, \theta, \varphi$

**Ensure:** Optimal control $u^*$ and optimal state $f^* = f(u^*)$

1. while $\|u_{l+1} - u_l\| > tol$ do
2. Solve forward equation $\partial_t f + \text{div}(a(x, t; u)f) = 0, f_{t=0} = f_0$
3. Solve backward equation $-\partial_t q - a(x, t; u) \cdot \nabla q = -\theta, q_{t=T} = -\varphi$
4. Solve linearized forward eq. $\partial_t \rho + \text{div}(a \rho) = -\text{div}(\hat{a}f), \rho(x)|_{t=0} = 0$
5. Solve linearized backw. eq. $\partial_t \hat{q} - a \cdot \nabla \hat{q} = -\alpha f + \delta a \cdot \nabla q, \hat{q}|_{t=T} = 0$
6. Assemble Jacobian (Hessian of original Problem) $J_f u_l$ and gradient $F_f$
7. Solve $(J_f u_l) d_l = -F_f(u_l)$ (with GMRES)
8. Find stepsize $\sigma_l$ (with e.g. Armijo line-search)
9. $u_{l+1} = u_l + \sigma_l d_l$
10. end while
11. return $(f(u_l), u_l)$

$H^1$ projection

$$
\begin{aligned}
\min_{\bar{u} \in H^1_T} & \quad f_P(u) := \frac{\gamma}{2} \|\bar{u} - u\|_{L^2_T}^2 + \frac{\nu}{2} \left\| \frac{d}{dt} (\bar{u} - u) \right\|_{L^2_T}^2 \\
\text{s.t.} & \quad \max(u_a - \bar{u}) = 0, \quad \max(\bar{u} - u_0) = 0
\end{aligned}
$$
Numerical experiment

We choose $\Omega = [-1, 1] \times [-1, 1]$

$$f_0(x) = \frac{C_0}{2\pi \sigma^2} \exp\left(-\frac{|x - x_0|^2}{2\sigma^2}\right).$$

where $x_0 = (-0.5, 0.5)$, $\sigma = 0.25$, and $C_0 = \frac{1}{10}$. By this choice, the value of $f_0$ at the boundary of $\Omega$ is of the order of machine precision.

Figure: Left: desired trajectory; right: parametric plot of $E[x]$.
The stochastic motion of a pedestrian

Consider the motion of an individual, subject to random perturbation, whose (planar) position at time $t$ is denoted with $X(t) \in \mathbb{R}^2$, and its velocity field (drift) is given by $u$. We have

$$dX(t) = u(X(t), t) \, dt + \sigma \, dW(t), \quad X(t_0) = X_0,$$

We assume that reflecting barriers keep the pedestrian in a region $\Omega \subset \mathbb{R}^2$. The corresponding FP equation is given by

$$\partial_t f(x, t) - \frac{\sigma^2}{2} \Delta f(x, t) + \nabla \cdot (u(x, t) f(x, t)) = 0, \quad f(x, 0) = f_0(x)$$

where $f_0$ denotes the distribution of the initial position $X_0$. The FP equation can be written in flux form $\partial_t f = \nabla \cdot F(f)$, where

$$F_j(x, t; f) = \frac{\sigma^2}{2} \partial_{x_j} f(x, t) - u_j(x, t) f(x, t).$$

Reflecting barriers correspond to flux zero boundary conditions $F \cdot n = 0$ on $\partial \Omega \times (0, T)$, where $n$ is the unit outward normal on $\partial \Omega$.

\textsuperscript{17} M. Annunziato and A. Borzì, Optimal control of probability density functions of stochastic processes, Mathematical Modelling and Analysis, 15 (2010), 393-407.
Ensemble control of the motion of one pedestrian

Consider the control of the motion of the pedestrian by the velocity field

\[
J(f, u) = \int_0^T \int_\Omega \theta(x, t) f(x, t) \, dx \, dt + \int_\Omega \varphi(x) f(x, T) \, dx \\
+ \frac{\nu}{2} \int_0^T \int_\Omega C(u(x, t)) \, dx \, dt,
\]

where \( \nu \geq 0 \).

In this setting, \( \theta \) represents an attracting (valley) and/or repulsive (soft obstacle) potential for the PDF. If \( x_D(t) = (x^1(t), x^2(t)) \) denotes a desired trajectory for the pedestrian, we may choose \( \theta(x, t) = |(x - x_D(t))|^2 \).

Similarly for \( \varphi(x) \).

The first two terms are expected value functionals

\[
\mathbb{E}[\int_0^T \theta(X(s), s) \, ds + \varphi(X(T)) \mid X(0) = X_0].
\]
We extend the construction of ensemble controls considering \( u = u(x,t) \), and the cost of the control is given by one of these two choices

\[
C(u(x,t)) = |u(x,t)|^2 \quad (I), \quad C(u(x,t)) = |u(x,t)|^2 f(x,t) \quad (II).
\]

This term determines the control space \( \mathcal{U} \) where the control is sought. In the first case, we have \( L^2(Q) \) costs \( (Q = \Omega \times (0,T)) \), in the second case \( u \) is required to be square-integrable in the measure induced by the process \( X(t) \).

In addition, we may require that the control belongs to an admissible set with point-wise constraints as the following

\[
U_{ad} = \{ u \in \mathcal{U}, \ u(x,t) \in K_U, \ \text{a.e. in } Q \}.
\]

Notice that the control mechanism is introduced at the ‘microscopic’ level in the SDE as a drift and this automatically appears in the FP model.
FP optimality system (I)

In the case of $L^2(Q)$ costs of the control (case (I)), the first-order optimality condition is given by the following optimality system (Lagrange function $L = J + \langle FPE, p \rangle$)

\[
\frac{\partial}{\partial t} f(x, t) - \frac{\sigma^2}{2} \Delta f(x, t) + \nabla \cdot (u(x, t) f(x, t)) = 0
\]

\[
F \cdot n = 0, \quad f(x, 0) = f_0(x)
\]

\[
-\frac{\partial}{\partial t} p(x, t) - \frac{\sigma^2}{2} \Delta p(x, t) - u(x, t) \cdot \nabla p(x, t) + \theta(x, t) = 0
\]

\[
\frac{\partial p}{\partial n} = 0, \quad p(x, T) = -\varphi(x)
\]

\[
\langle v u - f \nabla p, v - u \rangle \geq 0 \quad \forall v \in U_{ad}.
\]
FP optimality system (II)

In the case (II), the \textbf{optimality system} is given by (Lagrange function \( L = J - \langle FPE, p \rangle \))

\[
\partial_t f(x, t) - \frac{\sigma^2}{2} \Delta f(x, t) + \nabla \cdot (u(x, t) f(x, t)) = 0 \\
F \cdot n = 0, \quad f(x, 0) = f_0(x)
\]

\[
\partial_t p(x, t) + \frac{\sigma^2}{2} \Delta p(x, t) + u(x, t) \cdot \nabla p(x, t) + \theta(x, t) + \frac{v}{2} |u(x, t)|^2 = 0 \\
\frac{\partial p}{\partial n} = 0, \quad p(x, T) = \varphi(x)
\]

\[
\langle f(\nu u + \nabla p), \nu - u \rangle \geq 0 \quad \forall \nu \in U_{ad}.
\]

Consider this variational inequality pointwise, and notice that \( f > 0 \) a.e. in \( Q \). Then, it is sufficient \((\nu u + \nabla p) (\nu - u) \geq 0\), which characterizes the solution to \( \min_{\nu \in K_U} [\nu \cdot \nabla p + \frac{v}{2} |\nu|^2] \) at any point in \( Q \).
The Hamilton-Jacobi-Bellman equation

In case (II), we can consider the expected value functional\textsuperscript{20}

\[ J_{t_0, x_0}(u) = \mathbb{E}\left[ \int_{t_0}^{T} \theta(X(s), s) + \frac{\nu}{2} |u(X(s), s)|^2 ds + \varphi(X(T)) \mid X(t_0) = X_0 \right], \]

Correspondingly, we have the optimal control \( u^* = \arg\min_{u \in \mathcal{U}} J_{t_0, x_0}(u) \), and the so-called value function

\[ q(x, t) := \min_{u \in \mathcal{U}} J_{t, x}(u) = J_{t, x}(u^*), \]

which satisfies the HJB equation

\[ \partial_t q + H(x, t, \nabla q, \Delta q) = 0, \quad q(x, T) = \varphi(x), \]

with the Hamilton-Pontryagin function

\[ H(x, t, \nabla q, \Delta q) := \min_{v \in K_U} \left[ \frac{\sigma^2}{2} \Delta q(x, t) + v \cdot \nabla q(x, t) + \theta(x, t) + \frac{\nu}{2} |v|^2 \right]. \]

Numerical experiments

Consider a two-dimensional stochastic process

\[ dX_1(t) = u_1(X_1(t), X_2(t), t) \, dt + \sigma \, dW_1(t) \]
\[ dX_2(t) = u_2(X_1(t), X_2(t), t) \, dt + \sigma \, dW_2(t) \]

where \( X_1(t) \) and \( X_2(t) \) represent the coordinates of the position of the pedestrian confined in \( \Omega = (-L, L) \times (-L, L) \) with \( L = 6 \).

The initial PDF of the position is given by

\[ f_0(x) = \hat{C} e^{-\{(x_1-A_1)^2-(x_2-A_2)^2\}/0.5} \]

where \((A_1, A_2) = x_t(0)\) is the starting point of a desired trajectory \( x_D = (t, \sin(2t)), \ t \in [0, \pi], \) and \( \hat{C} \) is a normalization constant.

We set \( \nu = 10^{-2} \) and \( \sigma = 1 \). The bounds on the velocity control field are five by \( K_U = [u_a, u_b] \times [u_a, u_b] \) where \( u_a = -5 \) and \( u_b = 5 \).
Numerical experiments with (I) and (II)

FP approximation: alternate-direction implicit (ADI) scheme (time) combined with a Chang-Cooper (CC) method (space). This scheme is structure preserving and second-order accurate. FP adjoint approximation by discretize-before-optimize strategy, and projected NCG for optimization\textsuperscript{21, 22}

\begin{figure}
\centering
\includegraphics[width=0.4\textwidth]{figure1.png}
\includegraphics[width=0.4\textwidth]{figure2.png}
\caption{Left: the Monte-Carlo simulation corresponding to the control cost (I). Right: the Monte-Carlo simulation corresponding to the control cost (II).}
\end{figure}


Numerical experiments with a soft obstacle

A soft obstacle is modelled with a ‘concave’ potential function

$$\hat{\theta}(x, t) = \begin{cases} 100, & (x_1 - 3)^2 + x_2^2 \leq 0.2^2 \\ (x_1 - 1.5t)^2 + x_2^2, & \text{otherwise,} \end{cases}$$

This is a cylinder centred at $(3, 0)$ and radius 0.2.
Consider a desired trajectory given by $x_D = (1.5t, 0)$, and our initial PDF at the point $(0, 0)$. The time interval is $[0, 2]$.

(a) Actual trajectory

(b) Monte-Carlo with FP

Figure: Trajectories with an obstacle. Figure 3a shows the evolution of the PDF $f$. Figure 3b shows the Monte-Carlo simulation with control cost (I).
Open issues in the control of Boltzmann models

In the Lagrange framework, PDE control problems are solved based on first-order optimality conditions: the governing model, its adjoint counterpart, and a gradient equation (or inequality).

One immediately recognizes that the resulting adjoint BE model has not a kinetic structure. This is the case for linear and nonlinear BE models.

A kinetic structure is required in order to apply the direct simulation Monte Carlo (DSMC) method\(^{23}\) which is necessary in the regime of dilute gases.

We investigate these issues focusing on the Keilson-Storer (KS) master equation\(^{24}\)

This is a linear space-homogeneous BE model that has been successfully applied in, e.g., the estimation of transport coefficients, laser spectroscopy, and molecular dynamics simulations, reorientation of molecules in liquid water, and quantum transport.

---


Keilson-Storer master equation

Keilson-Storer master equation in velocity space with gain-term and loss-term

\[ \partial_t f(v, t) = \int f(w, t) A(w, v) \, dw - f(v, t) \int A(v, w) \, dw, \]

with collision kernel containing parameter \( \gamma \in [-1, 1] \)

\[ A(v, w) := A_0 \exp \left( -\beta |w - \gamma v|^2 \right), \quad A_0, \beta > 0. \]

We define the collision operator

\[ C[f](v, t) := \int f(w, t) A(w, v) \, dw - f(v, t) \int A(v, w) \, dw. \]

(Integrals are in the entire velocity space \( \mathbb{R}^d \))

Regimes:

- \( \gamma \ll 1 \): weak collisions, Brownian motion
- \( \gamma = 0 \): Bhatnagar–Gross–Krook operator
- \( \gamma \gg -1 \): re-orientation of molecules in liquid water, quantum transport
Details concerning the KS model & control

▶ proposed to model Brownian motion: species with different masses and densities, denote with $\Gamma = 1/\tau$ the inverse of the mean free time between collisions

▶ microscopic scattering is a ‘damping’ process; detailed balance is satisfied: $A(w, v) f^{eq}(w) = A(v, w) f^{eq}(v)$.

▶ The positive $A_0, \beta > 0$ are related by requiring that $f^{eq}(v) = f_0 \exp\left(-\beta (1 - \gamma^2) |v|^2\right)$ is the Maxwellian distribution and $\int A(v, w) dw = 1$. In 2D velocity space $A_0 = \Gamma \beta / \pi$, and $\beta (1 - \gamma^2) = \frac{M}{2k_B T}$.

Control mean velocity $\mu(t) = \langle v(t) \rangle := \mathbb{E}[v](t), t \in [0, T]$ using a control mechanism $u$ in the collision kernel:

$$\partial_t f(v, t) = C_u[f](v, t) := \int f(w, t) A(w, v; u) \, dw - f(v, t) \int A(v, w; u) \, dw,$$

$$A(v, w; u) := A_0 \exp\left(-\beta |w - \gamma v + u|^2\right), \quad A_0, \beta > 0, \gamma \in [-1, 1]$$
Keilson-Storer ensemble optimal control problem

The aim of our KS optimal control problem is to find an optimal control $u \in U = H^1_0(0, T)$ such that the variance of the velocity of each particle w.r.t. a desired velocity configuration $v_D(t), t \in (0, T)$, and $v_T$ at $t = T$, is minimized. We have\(^\text{25}\)

$$
\min_{u \in U} J(f, u) := \int_0^T \int \theta(v, t) f(v, t) \, dv \, dt + \int \phi(v)f(v, T) \, dv + \frac{\nu}{2} \|u\|^2_U
$$

s.t. $\partial_tf(v, t) = C_u[f](v, t), \quad f(v, 0) = f_0(v)$

with given $f_0, \theta, \phi$, and weight of the cost of the control $\nu > 0$. The resulting optimality system is given by

$$
\partial_tf(v, t) = C_u[f](v, t), \quad f(v, 0) = f_0(v)
$$

$$
- \partial_t q(v, t) = \bar{C}_u[q](v, t) - \theta(v, t), \quad q(v, T) = -\varphi(v)
$$

$$
- u''(t) + u(t) = \frac{1}{\nu} \int q(v, t) \partial_u C_u[f](v, t) \, dv, \quad u(0) = 0, u(T) = 0.
$$

\(^{25}\) J. Bartsch, A. Borzi, G. Nastasi, Optimal control of the Keilson-Storer master equation in a Monte Carlo framework.
The KS adjoint equation

In the KS adjoint equation, we have

\[ \tilde{C}_u[q](v, t) = \int A(v, w; u) q(w, t) \, dw - q(v, t) \int A(v, w; u) \, dw. \]

This operator has not a gain-loss structure. This structure can be partially recovered defining

- \( C_u^*[q](v, t) = \int A^*(w, v; u) q(w, t) \, dw - q(v, t) \int A^*(v, w; u) \, dw, \)
- \( A^*(w, v; u) = \frac{1}{\gamma} A(v, w; u) \)
- ‘adjoint’ mean free time \( \tau_q = \gamma \tau \)
- \( \int (A(w, v; u) - A(v, w; u)) \, dw = \Gamma \frac{1-\gamma}{\gamma} =: C_0^*. \)

We can write the adjoint KS equation as follows

\[ -\partial_t q(v, t) = C_u^*[q](v, t) + C_0^* q(v, t) - \theta(v, t). \]

This equation has the required kinetic structure, with the addition of a linear reaction term and a source term.
Approximation of the KS adjoint equation

In a probabilistic/kinetic framework, we can think of $\theta$ as a source or sink of particles if it can be interpreted as a density distribution. For this purpose, we choose

$$\theta(v, t) = -\frac{C_\theta}{2\pi\sigma_C^2} \exp \left( -\frac{|v - v_D(t)|^2}{2\sigma_C^2} \right), \quad \sigma_C = 1/\sqrt{2\beta};$$

and similarly for $\varphi$. It may be convenient to reverse time by the transformation $s := T - t$.

Having $f$ and $q$, we can assemble the reduced gradient

$$\nabla_u \hat{J}(u) \bigg|_{L^2}(t) = -v u''(t) + v u(t) - \int q(v, t) \partial_u C_u[f](v, t) \, dv.$$

Further, to obtain the $H^1$ representative of this gradient we use the fact that

$$(\nabla_u \hat{J}(u) \bigg|_{L^2}, \delta u)_{L^2} = (\nabla_u \hat{J}(u) \bigg|_{H^1}, \delta u)_{H^1}$$

for all $\delta u \in H^1$.

If the control is sought in $H^1_0(0, T)$, we solve

$$-\frac{d^2}{dt^2} \psi + \psi = \nabla_u \hat{J}(u) \bigg|_{L^2}, \quad \psi(0) = 0, \quad \psi(T) = 0.$$

(In the weak formulation.) Thus, $\nabla_u \hat{J}(u) \bigg|_{H^1} = \psi$. 

Alfio Borzì
Monte Carlo methods and optimization

Use the kinetic description of gas and split the solution operator.

**Free flight**

deterministic

\[ \dot{x} = v \]

\[ x(t + \Delta t) = x(t) + v\Delta t \]

**Collision**

probabilistic

\[ v_{after} \sim \mathcal{N}(\gamma v_{before} - u, \sigma^2) \]

*Box-Muller-method*

---

**Algorithm**

1. **Input**
   - \( u_0(t) \)
   - \( f_0(x,v) \)
   - \( \theta(x,v,t) \)
   - \( \phi(x,v) \)

2. **Initialize**
   - \( l = 0 \)

3. **Forward**
   - solve forward equation using DSMC
   - collision + pusher + control
   - \( f_l(x,v,t) \)
   - \( \Delta t \)

4. **Backward**
   - solve backward equation using DSMC
   - collision + pusher + control + \( \theta \)
   - \( q_l(x,v,t) \)
   - \( \Delta t \)

5. **Assemble gradient**
   - \( g_l \leftarrow f_l, q_l, u_l \)

6. **Update control**
   - \( u_{l+1} = u_l + \sigma_l d_l \)

7. **Diagnosis**
   - \( \langle v \rangle, \langle g \rangle_l, \langle J(u) \rangle_l, \ldots \)

8. **Check termination**
   - if \( c_l \) then \( l = l + 1 \)

---

**Remarks**

- Alfio Borzì
- On ensemble optimal control problems governed by Liouville, Fokker-Planck and linear Boltzmann equations
Physical setting

Initially the particles of mass \( m \) are at thermal equilibrium obeying the Boltzmann-Maxwell distribution at temperature \( \tilde{T} = \tilde{T}_0 > 0 \)

\[
f_0 = \mathcal{N}_2 \left( 0, \frac{k_B \tilde{T}_0}{m} I_2 \right),
\]

where \( k_B \) is the Boltzmann constant. For the mean collision frequency

\[
\Gamma = \frac{1}{\tau} = \frac{N_f}{V} \pi d^2 \langle v_r \rangle,
\]

where \( N_f \) is the number of particles, \( V \) the volume of the domain, \( d \) the effective diameter of the particle, and \( \langle v_r \rangle \) the average relative speed between particles. In the case of thermal equilibrium

\[
\langle v_r \rangle = \frac{4}{\sqrt{\pi}} \sqrt{\frac{k_B \tilde{T}^{st}}{m}}.
\]

Therefore we obtain

\[
\Gamma = 4 \frac{N_f}{V} d^2 \sqrt{\frac{\pi}{\beta}}, \quad \beta = \frac{m}{k_B \tilde{T}^{st}}, \quad \tilde{T}^{st} = \tilde{T}_0 (1 - \gamma^2),
\]

where \( \tilde{T}^{st} \) is the temperature of the steady state and \( \tilde{T}_0 \) the temperature of the initial state.
Experimental setting

We consider the ensemble optimal control problem in 2D:

\[ v_d(t) = \left( 250 \sin \left( \frac{2\pi}{T} t \right), \frac{V_{\text{max}}}{2T} t \right), \quad \theta(v, t) = -\frac{C_\theta}{2\pi\sigma^2_\theta} \exp \left( -\frac{|v - v_D(t)|^2}{2\sigma^2_\theta} \right), \]

\[ u^0(t) := (0, 0)^T, \quad \varphi(v) = -\frac{C_\varphi}{2\pi\sigma^2_\varphi} \exp \left( -\frac{|v - v_D(T)|^2}{2\sigma^2_\varphi} \right), \]

where \( C_\theta = 10^{20} \) and \( C_\varphi = 10^3 \), \( \sigma_\theta = \sigma_\varphi = 10\sigma = 10\sqrt{1/(2\beta)} \).

<table>
<thead>
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<th>Symbol</th>
<th>Value</th>
<th>Symbol</th>
<th>Value</th>
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<td>( m ) [kg]</td>
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<td>( k_B ) ( \frac{m^2 kg}{s^2 K} )</td>
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<td>( d ) [m]</td>
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</tr>
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<td>( T ) [s]</td>
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</tr>
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</table>

**Table**: Physical and numerical parameters.
Convergence history of $J$, optimal control field; comparison between mean velocity (circle-line) and desired one (line). Left: $x$ component; right: $y$ component of the velocity.
Numerical experiments - $L^2$

Convergence history of $J$, optimal control field; comparison between mean velocity (circle-line) and desired one (line). Left: $x$ component; right: $y$ component of the velocity.
Thank you

Thank you for your interest in this work!