Supervised learning for high-dimensional mean-field optimal control

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Overview

Learning and control problems for interacting agent systems

Control and learning of *interacting agent systems* can be used to improve the **emergence** of collective behaviors, or to **enforce** specific desired states.

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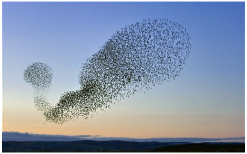

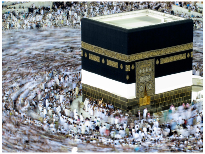

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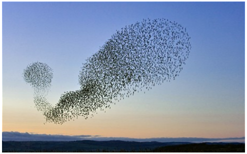
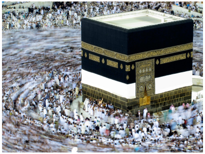
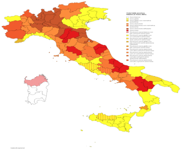




... but also influencing **consumers** towards a given good, **opinions**, over social networks, or (ideally) to prevent the spread of **infectious diseases**.





Optimization across scales

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  Hence we want to reduce the problem complexity introducing a mean-field description. [2]
- In this direction large interest has been shown to the so called mean-field optimal control and mean-field games in several **mathematical fields** (game theory, stochastic processes, analysis of PDEs, optimal control. . .), and in many **applications** (consensus or milling enforcement, evacuation problems, optimal taxation, network formation, vaccination strategies . . .). [3]

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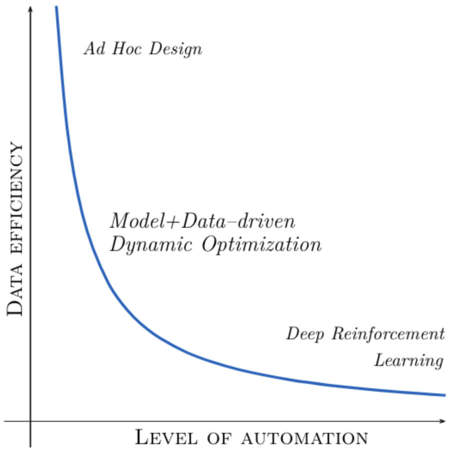
Computational optimization in a data-driven environment



Develop **feedback laws** for high-dimensional nonlinear dynamics

- employ efficient data-driven approaches (MPC, ANNs, PINNs,. . .)
- enhance : robustness and real-time computability.
- promote **sparse control action**.

High-dimensional optimal control

Let $(x_i(t), v_i(t))_{i=1}^N \in \Omega^N \subseteq \mathbb{R}^{2d\times N}$ evolves accordingly to

$$\frac{d}{dt}x_i = v_i$$

$$\frac{d}{dt}v_i = S(v_i) + \frac{1}{N}\sum_{j=1}^{N} H(x_i, x_j)(v_j - v_i) + \frac{1}{N}\sum_{j\neq i}\nabla W(|x_i - x_j|) + u_i$$

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- $S(v)$ is a **self-propulsion friction** term, e.g. $S(v) = (\alpha - \beta|v|^2)v$ for $t \to \infty$ gives us the desired velocity of the system $|v| = \sqrt{\alpha/\beta}$.

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- $H(\cdot)$ is alignment kernel, e.g.

$$H(r) = (1 + r^2)^{-\beta}; \beta \geq 0$$

- $W(\cdot)$ is a attraction-repulsion kernel interaction, e.g. of **power law** potential type

$$W(r) = r^a/a - r^b/b, a > b > 0.$$

- $u = (u_1, \dots, u_N) \in \mathbb{R}^{d\times N}$ is a stabilizing/control term,

$$u^* = \arg\min \int_0^T \frac{1}{N}\sum_{i=1}^{N} \left(|\bar{v} - v_i|^2 + \gamma|u_i|^2\right) dt$$

Swarming dynamics

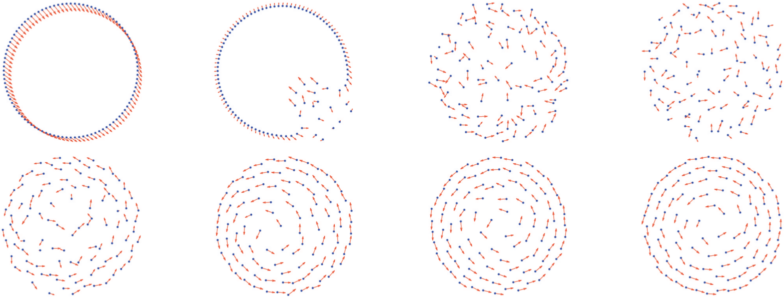

Figure – Transition from unstable flocking to stable milling.

Swarming dynamics

High-dimensional optimal control

Microscopic optimal control

$$V(x,v,t_0) := \min_{u\in\mathcal{U}^N} J^N(u;x,v,t_0) := \int_{t_0}^{T} \underbrace{\frac{1}{N}\sum_{i=1}^{N}\ell(x_i(t),v_i(t))}_{L(x(t),v(t))} + \gamma\sum_{i=1}^{N}|u_i(t)|^2 dt$$

$$s.t. \quad \dot{x}_i = v_i, \quad \dot{v}_i = F_i(x,v) + u_i, \qquad i = 1,\dots,N$$

4. Richard E. Bellman, '57

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Optimal feedback law : $u^* = -\frac{1}{2\gamma}\nabla_v V(x,v,t)$

Hamilton-Jacobi-Bellman PDE

$$\partial_t V(x,v,t) - \frac{1}{4\gamma}\left(|\nabla_x V(x,v,t)|^2 + |\nabla_v V(x,v,t)|^2\right)$$
$$+ v\cdot\nabla_x V(x,v,t) + F(x,v)\cdot\nabla_v V(x,v,t) + L(x,v) = 0, \quad V(x,v,T) = 0$$

Curse of dimensionality.[4] For $N, d \gg 1$ the computational effort renders the problem unsolvable.

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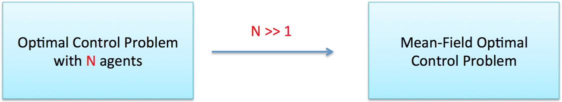
Mean-field optimal control



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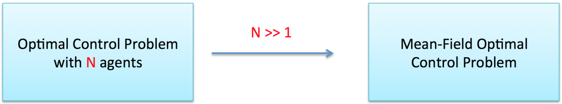

Mean-field optimal control [5]

Denote $f = f(x, v, t)$ the density of particles and the control $u = u(x, v, t)$, thus (f, u) is obtained as follows

$$\min_{u \in \mathcal{U}_\ell} J(u; f^0) := \int_0^T \int_{\mathbb{R}^{2d}} \left(|\bar{v} - v|^2 + \gamma \psi(u) \right) f(x, v, t)\, dx\, dv\, dt$$

$$s.t. \quad \partial_t f + v \cdot \nabla_x f = -\nabla_v \cdot ((\mathcal{F}[f] + u) f), \qquad f(x, v, 0) = f^0(x, v).$$

where

$$\mathcal{F}[f](x, v, t) = \int_{\mathbb{R}^{2d}} F(x, v, y, w) f(y, w)\, dy\, dw.$$

and $\psi(\cdot)$ is a non-negative convex penalization function.

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Mean-field optimal control (first order optimality)

First order optimality conditions[6]

$$\partial_t f + v \cdot \nabla_v f = -\nabla_v \cdot \left((\mathcal{F}[f] + u) \, f \right),$$
$$\partial_t p + v \cdot \nabla_v p = |\bar{v} - v|^2 + \gamma\psi(u) - (\mathcal{F}[f] + u) \cdot \nabla_v p - \mathcal{G}[f,p]$$
$$\gamma \nabla_u \psi(u) - \nabla_v p = 0,$$

with initial data $f(x,v,0) = f^0(x,v)$ and terminal condition $p(x,v,T) = 0$ and where

$$\mathcal{G}[f,p](x,v,t) = \int_{\mathbb{R}^{2d}} F(y,x,w,v) \cdot \nabla_v p(y,w,t) f(y,w,t) \, dydw.$$

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- Derivation of optimality conditions in Wasserstein metric[7].

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Numerical realization of mean field optimal control

Consider the following functional with quadratic penalization $\psi(u) = |u|^2$

$$\min_{u\in\mathcal{U}_\ell} J(u; f^0) := \int_0^T \int_{\mathbb{R}^{2d}} \left(|v-\bar{v}|^2 + \gamma|u|^2\right) f(x,v,t)\, dx\, dv\, dt,$$

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Reduced gradient method

1. Set the initial guess $u^0(v,t) = 0$, tolerance `tol` and $k = 0$
2. `while` $|\nabla J(u^k) - \nabla J(u^{k-1})| \geq$ `tol`
   - Solve the **forward equation** with u^k for f^k ;
   - Solve the **backward equation** with u^k, f^k for p^k ;
   - Update $u^{k+1} = u^k + \alpha_k \nabla J(u^k)$;

     → $\nabla J(u^k) = 2\gamma u^k - \nabla_v p^k$ and α_k descent step.
   - $k = k + 1$.

   `end while`

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Substituting the $2\gamma u^k - \nabla_v p^k = 0$ into the backward equation restitutes a non-local HJ- equation

$$\partial_t p = |\bar{v} - v|^2 - \frac{1}{4\gamma}|\nabla_v p|^2 - \mathcal{F}[f]\cdot\nabla_v p - \mathcal{G}[f,p] + \sigma D(v)\Delta_v p$$

Optimal control of mean-field Cucker-Smale

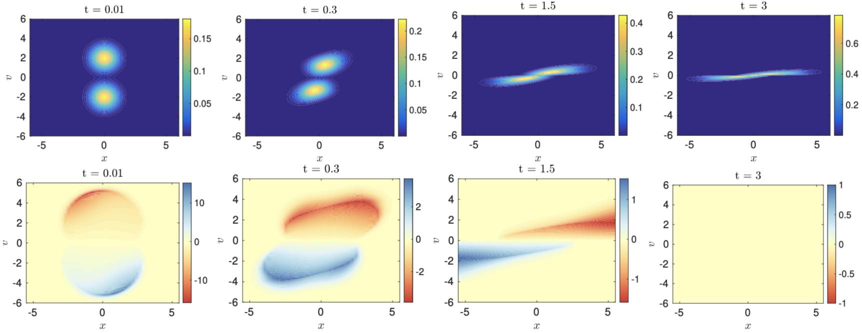
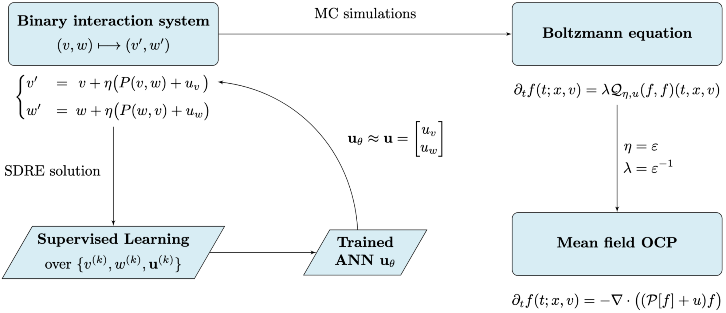


Figure – Cucker-Smale model : $F(x, v, y, w) = H(|x - y|)(w - v)$. Top : evolution of the forward model $f(x, v, t)$. Bottom : evolution of the control $u(x, v, t)$.

Taming c.o.d. via supervised kinetic control



(Sub)-optimal binary approach

- Introduce the **discrete binary interaction model**

$$v_i^{m+1} = v_i^m + \Delta t F(x_i^m, v_i^m, x_j^m, v_j^m) + \Delta t u_i^m,$$
$$v_j^{m+1} = v_j^m + \Delta t F(x_j^m, v_j^m, x_i^m, v_i^m) + \Delta t u_j^m,$$

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- Design a **functional** associated to the discrete binary dynamics

$$J_M(u_{ij}; v_{ij}^0) := \sum_{m=0}^{M-1} \int_{t_m}^{t_{m+1}} L\left(v_{ij}(t), u_{ij}(t)\right)\, dt,$$

where $v_{ij}(t) = (v_i(t), v_j(t))$, $u_{ij}(t) = (u_i(t), u_j(t))$, and

$$L(v_{ij}; u_{ij}) = |v_i - \bar{v}|^2 + |v_j - \bar{v}|^2 + \gamma\left(\psi(u_i) + \psi(u_j)\right).$$

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(Sub)-optimal binary approach

- Introduce the **discrete binary interaction model**

$$v_i^{m+1} = v_i^m + \Delta t F(x_i^m, v_i^m, x_j^m, v_j^m) + \Delta t u_i^m,$$
$$v_j^{m+1} = v_j^m + \Delta t F(x_j^m, v_j^m, x_i^m, v_i^m) + \Delta t u_j^m,$$

- Design a **functional** associated to the discrete binary dynamics

$$J_M(u_{ij}; v_{ij}^0) := \sum_{m=0}^{M-1} \int_{t_m}^{t_{m+1}} L\left(v_{ij}(t), u_{ij}(t)\right)\, dt,$$

where $v_{ij}(t) = (v_i(t), v_j(t))$, $u_{ij}(t) = (u_i(t), u_j(t))$, and

$$L(v_{ij}; u_{ij}) = |v_i - \bar{v}|^2 + |v_j - \bar{v}|^2 + \gamma\left(\psi(u_i) + \psi(u_j)\right).$$

- Compute the optimal feedback control for the reduced problem [8]

$$u_i^m = K_{\Delta t}(t_m, x_i, v_i, x_j, v_j), \quad u_j^m = K_{\Delta t}(t_m, x_j, v_j, x_i, v_i)$$

8. G.A., M. Herty, L. Pareschi, M. Zanella '14-'15 ;G.A., Y. Choi, M. Fornasier, D. Kalise '17-'19 ; G.A., S. Bicego, D. Kalise '21-'22.

A Boltzmann-like model

We consider the binary dynamics where we assume that two individuals modify their states, after the interaction, according to

$$v' = v + \alpha F(x, v, y, w) + \alpha K_\alpha(t, x, v, y, w)$$
$$w' = w + \alpha F(y, w, x, v) + \alpha K_\alpha(t, y, w, x, v)$$

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- v^*, w^* are the **post-interaction** velocities,
- α is a parameter that measures the **strength of the interactions**
- For example in the case of **instantaneous control** we have

$$K_\alpha(x,v,y,w) = \frac{\alpha}{\gamma + \alpha^2}\left((\bar{v} - v) - \alpha F(x,v,y,w)(w-v)\right).$$

A Boltzmann-like model

We denote with $f = f(x, v, t)$ the density of individuals at time t. Thus the density f is solution of the following Povzner-Boltzmann-type equation

$$\partial_t f + v \cdot \nabla_x f = \lambda Q_{\alpha,\gamma}(f, f),$$

$$Q_{\alpha,\gamma}(f, f) = \int_{\mathbb{R}^{2d}} \left(\frac{1}{J_\kappa} f(x, v_*) f(y, w_*) - f(v) f(w) \right) dy\, dw,$$

Where $('v,' w)$ are the **pre-interaction** states and J_κ is the Jacobian of the transformation $(v, w) \to (v', w')$. The Boltzmann-type operator in its **weak form** reads

$$\lambda \langle Q_{\alpha,\gamma}(f, f), \varphi \rangle = \lambda \iint_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} \left(\varphi(x, v') - \varphi(x, v) \right) f(x, v) f(y, w) dx dv\, dy dw.$$

Grazing-collision limit

Theorem (Costrained grazing-collision limit)

Let us fix a control $U_{\alpha,\gamma} \in \mathcal{U}$, $F(\cdot) \in L^2_{loc}$. For $\varepsilon > 0$, the *grazing-collision scaling*[9] reads as follows

$$\alpha = \varepsilon, \qquad \lambda = \frac{1}{\varepsilon}$$

and define $f^\varepsilon(x, v, t)$ as a solution of the Boltzmann-like equation. Then, for $\varepsilon \to 0$, $f^\varepsilon(x, v, t)$ converges pointwise to a solution of the "mean-field controlled equation of the microscopic model, namely

$$\partial_t f + v \cdot \nabla_x f = -\nabla_v \cdot ((\mathcal{F}[f] + \mathcal{K}[f])\, f),$$

where

$$\mathcal{F}[f](x, v, t) = \int_{\mathbb{R}^{2d}} F(x, v, y, w) f(y, w, t)\, dydw,$$

$$\mathcal{K}[f](x, v, t) = \int_{\mathbb{R}^{2d}} K(x, v, y, w, t) f(y, w, t)\, dydw.$$

Where for $\varepsilon \to 0$, $K_\varepsilon(x, v, y, w, t) \to K(x, v, y, w, t)$ is well defined.

9. Toscani '06, Villani '98.

Offline phase
approximated controlled binary interactions

- Sample paired interacting agents, numerically solve the controlled binary OCP and generate training dataset.
- Train the FNN to approximate the feedback laws $u_\theta, u_V \approx u$

Online phase
Monte Carlo simulation of the evolving pdf

- At each discrete time t_h, coupled interacting agents are randomly sampled from the current distribution $f(t_h, x)$.
- For each couple, compute the u_θ/u_V-controlled post-interaction states.
- The updated agent distribution $f(t_{h+1}, x)$ is approximated as the sampling distribution of the post-interaction states.

Stochastic simulation methods

Goal : Simulate the binary constrained interaction dynamics with small values of ε in order to approximate the original microscopic model.

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- We use a **splitting method**, evaluating in two different steps the transport and collisional part of the scaled Boltzmann equation

$$\frac{\partial f}{\partial t} = -v \cdot \nabla_x f \tag{T}$$

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} Q_\varepsilon(f, f) \tag{C}$$

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- We define $f^n = f(x, n\Delta t)$, and we consider the foward discretization of the collisional step

$$f^{n+1} = \left(1 - \frac{\Delta t}{\varepsilon}\right) f^n + \frac{\Delta t}{\varepsilon} Q_\varepsilon^{+,n}(f^n, f^n)$$

$$v^{n+1} = v^n + \Delta t F(x^n, v^n, y^n, w^n) + \Delta t K_{\Delta t}(x^n, v^n, y^n, w^n)$$
$$w^{n+1} = w^n + \Delta t F(y^n, w^n, x^n, v^n) + \Delta t K_{\Delta t}(y^n, v^n, x^n, w^n)$$

Accuracy and efficiency

- Precompute the feedback control law $K_{\Delta t}(\cdot, \cdot)$.

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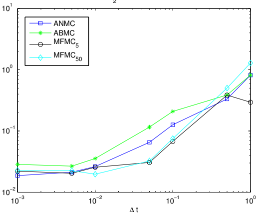
- Collocation methods of order k have accuracy $O(N^{-k/d})$. DSMC methods are more efficient if $k \leq d/2$.
- The resulting algorithm is **fully meshless**.[b].

$N_s = 10^5$



Instantaneous control

We reduce the original optimization into the minimization of

$$J_{\Delta t} = \left(|v_i^{m+1} - \bar{v}|^2 + |v_j^{m+1} - \bar{v}|^2 \right) + \gamma \left(|u_i^m|^p + |u_j^m|^p \right).$$

Thus the minimizers of the binary system are obtained as

$$u_i^*(v_i, v_j) = \mathcal{S}^p_{\gamma,\Delta t}(\xi_{ij}), \qquad u_j^*(v_i, v_j) = \mathcal{S}^p_{\gamma,\Delta t}(\xi_{ji}),$$

where

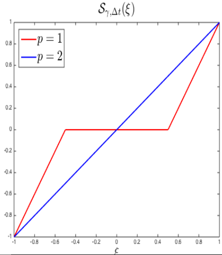
$$\xi_{ij}(v_i, v_j) \equiv (\bar{v} - v_i^m) - \frac{\Delta t}{2} P(v_i^m, v_j^m)(v_j^m - v_i^m), \qquad \xi_{ji} \equiv \xi_{ij}(v_j, v_i)$$

- For $p = 2$ we have

$$\mathcal{S}^2_{\gamma,\Delta t}(\xi) = \frac{\Delta t}{\gamma + \Delta t^2} \xi$$

- For $p = 1$ we have

$$\mathcal{S}^1_{\gamma,\Delta t}(\xi) := \begin{cases} \frac{1}{\Delta t} \left(1 - \frac{\gamma}{\Delta t |\xi|} \right) \xi, & |\xi| > \gamma/\Delta t\,, \\ 0 & otherwise \end{cases}$$



Finite horizon control

$$V(v_{ij}, t_m) := \inf_{u_{ij} \in \mathcal{U}^2} \sum_{k=m}^{M-1} \Delta t L(v_{ij}(t_k), u_{ij}(t_k)), \qquad \text{for } m = 0, \dots, M-1,$$

with terminal condition $V(v_{ij}, t_M) = 0$.

10. A. Alla, M. Falcone, D. Kalise '15.

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Efficient solution via **policy iteration** [10] for moderate dimensionality $d \in \{1, 2\}$,

$$V(v_{ij}, t_m) = \inf \left\{ V(v_{ij}^{+}(u_{ij}), t_{m+1}) + \Delta t L(v_{ij}, u_{ij}) \right\}, m = M-1, \dots, 0.$$

where $v_{ij}^{+}(u_{ij})$ is a one-step update of the binary controlled dynamics. Thus

$$(u_i^*(t_m), u_j^*(t_m)) = \arg\min_{u_{ij} \in \mathcal{U}^2} \left\{ V(v_{ij}^{+}(u_{ij}), t_{m+1}) + \Delta t L(v_{ij}, u_{ij}) \right\}. \qquad \text{(FH)}$$

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Infinite horizon control

State Dependent LQR

$$V(v_{ij}) := \inf_{u_{ij}\in\mathcal{U}^2} \Delta t \sum_{m=0}^{M-1} L(v_{ij}^m, u_{ij}^m) \approx \Delta t \sum_{m=0}^{M-1} (v_{ij}^m)^\top Q v_{ij}^m + (u_{ij}^m)^\top R u_{ij}^m$$

$$s.t. \quad v_{ij}^{m+1} = A_{\Delta t}(v_{ij}^m) v_{ij}^m + B_{\Delta t}(v_{ij}^m) u_{ij}^m,$$

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$$A_m = \begin{pmatrix} (1-\Delta t F_{ij}^m)\mathbb{I}_d & \Delta t F_{ij}^m \mathbb{I}_d \\ \Delta t F_{ij}^m \mathbb{I}_d & (1-\Delta t F_{ij}^m)\mathbb{I}_d \end{pmatrix}, \qquad B = \Delta t \mathbb{I}_{2d}$$

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$$u_{ij}^m = -K_m v_{ij}^m; \quad K_m = (R + B_m^\top \Pi_m B_m)^{-1} B_m^\top \Pi_m A_m; \qquad \Pi_m \in \mathbb{R}^{2d\times 2d}$$

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Discrete State Dependent Riccati Equation (dSDRE)

$$\Pi_m = Q + A_m^\top \Pi_m A_m - A_m^\top \Pi_m B_m (R + B_m^\top \Pi_m B_m)^{-1} B_m^\top \Pi_m A_m$$

Efficient approximation is performed in a MPC framework for large d.

Supervised learning approximation

NNs approximation

Compute the high-dimensional **feedback control** $u_\theta(v_{ij})$ exploiting the universal approximation property of NNs models [11]

11. Cybenko,'89 Hornik et al. '89-'91

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Compute the high-dimensional **feedback control** $u_\theta(v_{ij})$ exploiting the universal approximation property of NNs models [11]

- **Sampling data**. Sampled N_p pairs in $\mathbb{R}^d \times \mathbb{R}^d$ of interacting agents

$$\mathcal{S} = \{v_{ij}^k = (v_i, v_i)^{(k)}\}_{k=1}^{N_p},$$

and solve in an offline phase the **frozen SDREs** for $\mathcal{S}$.

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- **Generate synthetic data** $\mathcal{T}_u = \{v_{ij}^{(k)}, u(v_{ij}^{(k)})\}_{k=1}^{N_p}$ where

$$u(v_{ij}^{(k)}) = -\frac{R^{-1}B^T\nabla V(v_{ij}^{(k)})}{2} = -R^{-1}B^T\nabla V(v_{ij}^{(k)})\Pi_k v_{ij}^{(k)}. \qquad (1)$$

where, based on SDRE rappresentation, we make the ansatz

$$V(v_{ij}^{(k)}) = v_{ij}^{(k)\top}\Pi_k v_{ij}^{(k)}, \qquad \nabla V(v_{ij}^{(k)}) \approx 2\Pi_k v_{ij}^{(k)}.$$

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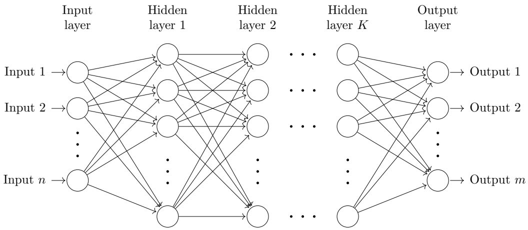
Supervised learning approximation

- We construct a feedforward NN to approximate the optimal feedback map



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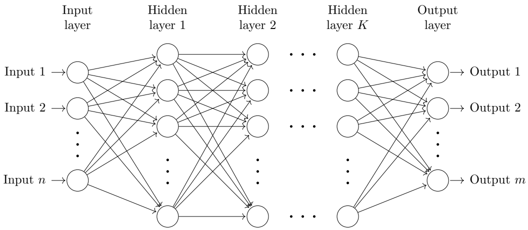

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- The parameters $\theta = \{W_r, b_r\}_r$ are trained by **minimizing the loss function**

$$\theta = \arg\min_\theta MSE(u, u_\theta^{FNN}) := \frac{1}{N_p}\sum_{k=1}^{N_p} \|u(v_{ij}^{(k)}) - u_\theta^{FNN}(v_{ij}^{(k)})\|^2$$

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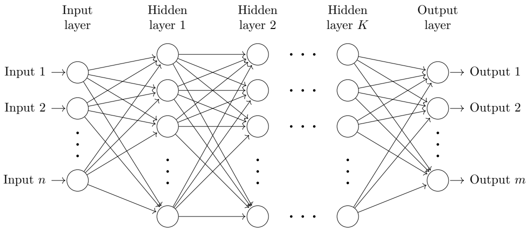

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- The number K of layers and neurons, the activation functions $\sigma_m(\cdot)$ are **hyper-parameters** of the model optimally tuned via a grid search in the parameter space by maximizing the precision of the trained model, by means of minimization of the mean relative error (MRE).

Consensus problem for swarming models $d_v = 15$

- The FNN has $K = 3$ hidden layers with 100 neurons per layer, and $\sigma(z) = max(0, z)$.
- Other approaches : **Recurrent NNs** (RNNs), and using NNs for the full **controlled state dynamics** $s^*_\theta = (x^*_{ij}, v^*_{ij})$.

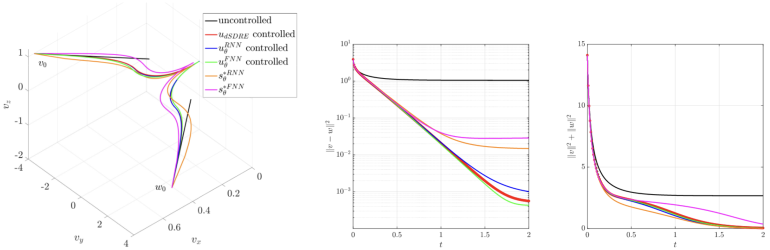

Figure – Evolution of the two interacting agents' restricted to the first 3 dimensions (left), decay to consensus (centre), and energy decay (right).

Optimal control of mean-field Cucker-Smale model

$Model$	s_θ^{*FNN}	s_θ^{*RNN}	u_θ^{FNN}	u_θ^{RNN}
r^2	0.99998	0.99999	0.99996	0.99998
MSE	0.075252	0.0069192	0.045596	0.018018

Table – Coefficient of determination r^2, MSE and mean percentage error over a collection of sampled states for dimension $d = 15$ and $N_p = 10^5$.

$d = 15$	$N_p = 10^2$	$N_p = 10^3$	$N_p = 10^4$	$N_p = 10^5$
u_θ^{FNN}	0.293578	2.447205	21.754862	2.2594×10^2
u_{dSDRE}	2.3866×10^2	2.3738×10^3	–	–
$N_s = 10^4$	$d = 3$	$d = 7$	$d = 15$	$d = 30$
u_θ^{FNN}	7.712628	11.006977	21.754862	70.172311
u_{dSDRE}	1.1979×10^3	5.2136×10^3	–	–

Table – CPU times (seconds) for the pair of agents in $\mathbb{R}^{4d}$, when considering different number of samples and dimensions. MC simulation parameters : $\Delta t = \epsilon = 0.01, T = 1$. The omitted records exceeded a time threshold $t_{max} = 24h$.

Control of mean-field swarming model ($N_s = 10^5, d = 3$)

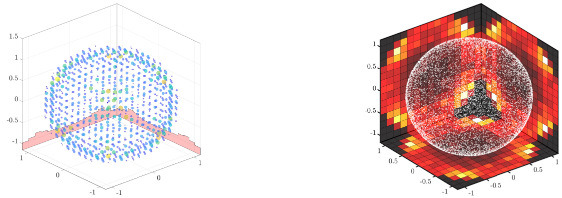

Figure – Uncontrolled dynamics in space and velocity.

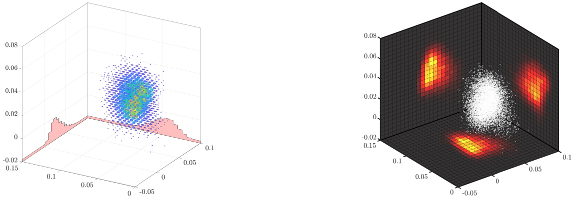

Figure – Controlled dynamics in space and velocity with u_θ^{FNN}. MC simulation parameters : $\Delta t = \epsilon = 0.02, T = 2$.

Conclusions

Conclusions & Perspectives

- Kinetic approximation of mean-field optimal control problems have been studied in [12]. Here, we introduced **supervised learning** approach to learn efficiently the control for high-dimensional systems. [13]

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3. We developed efficient exponential integrator schemes for mean-field optimal control problems (joint with M. Caliari, F. Cassini, E. Calzola).

12. G. A., M. Herty, L. Pareschi, M. Zanella, '13-'15-'19 ; G. A., D. Kalise, Y.-Choi, M. Fornasier '16-'17

13. G.A., S. Bicego, D. Kalise. '21-'22.

Conclusions & Perspectives

- Kinetic approximation of mean-field optimal control problems have been studied in [12]. Here, we introduced **supervised learning** approach to learn efficiently the control for high-dimensional systems. [13]

Further directions :

1. Mean-field optimal control for **multi-population dynamics** with transient leadership (joint with S. Almi, M. Morandotti, F. Solombrino and joint with F. Ferrarese).
2. Control of high-dimensional systems in **presence of uncertainties** . (joint with C. Segala, M. Herty)
3. We developed efficient exponential integrator schemes for mean-field optimal control problems (joint with M. Caliari, F. Cassini, E. Calzola).

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Thank for the attention !

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