

Inferring Interaction Rules from Observations of Evolutive Systems

(joint work with M. Fornasier, M. Hansen and M. Maggioni)



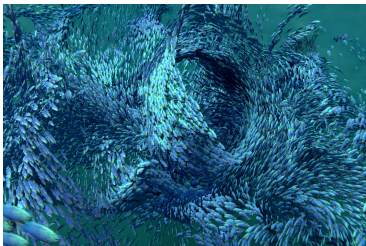
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Data-Rich Phenomena
Cambridge
December 14-16, 2015

What is a self-organizing system?



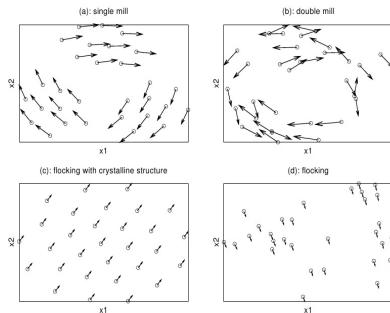
A framework for social dynamics

We consider multiagent systems
of the form: for $i = 1, \dots, N$

$$\dot{x}_i = \frac{1}{N} \sum_{j=1}^N a(|x_i - x_j|)(x_j - x_i) \in \mathbb{R}^d,$$

and their mean-field limit equation (here $F[a](\xi) = -a(|\xi|)\xi$)

$$\frac{\partial \mu}{\partial t} = -\nabla \cdot ((F[a] * \mu)\mu),$$



*Patterns related to different
balances of social forces*

Several “social forces” encoded in the **interaction kernel a** :

- alignment;
- repulsion-attraction;
- self-propulsion/friction...

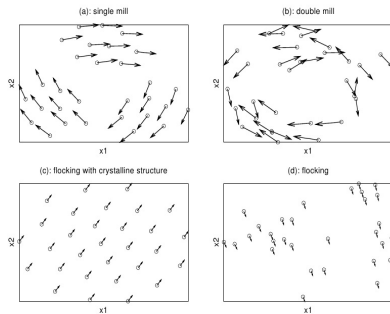
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The problem

- Tremendous theoretical success but the issue of actual applicability is so far scarcely addressed;
- Purely **qualitative analysis** to reproduce macroscopical patterns;
- Well-posedness relies on smoothness and asymptotic properties of the kernel a at 0 and ∞ ;
- Certainly results of great importance, as such functions likely differ from physical models: it is legitimate to consider a **large variety of function classes**;
- However, a solid mathematical framework on ‘learnability’ of interactions from observations of the dynamics **is not yet available**.

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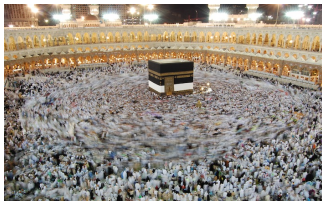
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$$\Rightarrow a(r) = \sin \left(\log(r + 1) \prod_{i=1}^d e^{\cos(i \cdot r^2)} + \dots \right)$$

The *naive* approach: optimal control

Given a **finite time horizon** $T > 0$ one would seek for a minimizer \hat{a} of

$$\mathcal{E}(\hat{a}) = \frac{1}{T} \int_0^T [\|x[a](s) - x[\hat{a}](s)\|^2 + \mathcal{R}(\hat{a})] ds,$$

being \mathcal{R} a suitable regularization functional and $t \mapsto x[\hat{a}](t) = (x_1(t), \dots, x_N(t))$ be the solution of

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However, one faces several problems!

- $t \mapsto x[\hat{a}](t)$ strongly nonlinear $\Rightarrow \mathcal{E}(\hat{a})$ strongly nonconvex;
- computationally unfeasible for N large (curse of dimensionality - Richard E. Bellman).

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The variational approach

Instead of minimizing the distances between trajectories $x[\hat{a}](t)$, we minimize the discrepancy between velocities $\dot{x}_i(t)$,

$$\mathcal{E}_N(\hat{a}) = \frac{1}{T} \int_0^T \frac{1}{N} \sum_{i=1}^N \left| \frac{1}{N} \sum_{j=1}^N \hat{a}(|x_i(t) - x_j(t)|) (x_i(t) - x_j(t)) - \dot{x}_i(t) \right|^2 dt,$$

among all functions

$$\hat{a} \in X = \{b : \mathbb{R}_+ \rightarrow \mathbb{R} \mid b \in L_\infty(\mathbb{R}_+) \cap W_{\infty,loc}^1(\mathbb{R}_+)\}$$

(ODEs and mean-field equations are well-posed).

Proposition

If $a, \hat{a} \in X$ then there exist a constant $C > 0$ depending on T, \hat{a} and $x_{0,1}, \dots, x_{0,N}$ and a “certain” compact set $K \subset \mathbb{R}_+$ such that

$$\|x[a](t) - x[\hat{a}](t)\| \leq C \sqrt{\mathcal{E}_N(\hat{a})} \quad \text{for all } t \in [0, T].$$

Hence, minimizing $\mathcal{E}_N(\hat{a})$ implies an accurate approximation of $t \mapsto x[\hat{a}](t)$ at finite time. (Proof: just a Gronwall.)



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The main question

- \mathcal{E}_N is easily computable from the knowledge of the trajectories of the system $x[a](t)$ (perhaps approximating $\dot{x}_i(t)$ by $\frac{x_i(t+\delta t) - x_i(t)}{\delta t}$).
- We use the number of agents N as an **optimization parameter**: does a larger number of agents improve learnability?
- Being quadratic (its minimization is just a least squares!!!), its minimizers can be **efficiently numerically computed** on a finite dimensional space $V_N \subset X$ such that $V_N \nearrow X$ as $N \rightarrow +\infty$.

Question: for which sequence V_N do minimizers

$$\hat{a}_N \in \operatorname{argmin}_{\hat{a} \in V_N} \mathcal{E}_N(\hat{a})$$

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Γ -limit of the \mathcal{E}_N

- Suppose there exists a functional \mathcal{E} such that $a = \operatorname{argmin}_{\hat{a} \in X} \mathcal{E}(\hat{a})$.
- Then the above question translates into the convergence of the minimizers of \mathcal{E}_N to the minimizer of \mathcal{E} , i.e., the Γ -convergence of \mathcal{E}_N to \mathcal{E} . But what can \mathcal{E} be?
- Set $F[a](\xi) = -a(|\xi|)\xi$ and rewrite the initial system as

$$\begin{cases} \dot{x}_i^N(t) = \frac{1}{N} \sum_{j=1}^N F[a](x_i^N(t) - x_j^N(t)) & \text{for } t \in (0, T], \\ x_i^N(0) = x_{0,i}^N, \end{cases} \quad i = 1, \dots, N.$$

- Define the empirical measure $\mu^N : [0, T] \rightarrow \mathcal{P}_c(\mathbb{R}^d)$ as

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A possible solution: the continuity equation

- μ^N is a solution to the **continuity equation** (abbreviated **c.e.**)

$$\frac{\partial \mu}{\partial t}(t) = -\nabla \cdot ((F[a] * \mu(t))\mu(t)) \quad \text{for } t \in (0, T].$$

with initial datum $\mu^N(0) = \mu_0^N := \frac{1}{N} \sum_{i=1}^N \delta_{x_{0,i}^N}$.

- Moreover, we can now rewrite \mathcal{E}_N as

$$\begin{aligned} \mathcal{E}_N(\hat{a}) &= \frac{1}{T} \int_0^T \frac{1}{N} \sum_{i=1}^N \left| \frac{1}{N} \sum_{j=1}^N (F[\hat{a}] - F[a])(x_i - x_j) \right|^2 dt \\ &= \frac{1}{T} \int_0^T \int_{\mathbb{R}^d} \left| (F[\hat{a}] - F[a]) * \mu^N(t) \right|^2 d\mu^N(t)(x) dt, \end{aligned}$$

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Existence and uniqueness of solutions of the c.e.

Theorem

- Suppose $a \in X$, let $T > 0$ and fix $\mu_0 \in \mathcal{P}_c(\mathbb{R}^d)$.
- Let μ be a weak solution of the c.e. with $\mu(0) = \mu_0$ on $[0, T]$.
- Let $\mu_0^N = \frac{1}{N} \sum_{i=1}^N \delta_{x_{0,i}^N}$ be such that $x_{0,i}^N \sim \mu_0$ i.i.d. $\forall N$ and $\forall i$.

Then, $\exists R > 0$ depending only on T, a , and $\text{supp}(\mu_0)$ such that it holds

$$\text{supp}(\mu^N(t)) \cup \text{supp}(\mu(t)) \subseteq B(0, R), \forall N \in \mathbb{N} \text{ and } \forall t \in [0, T],$$

$$\lim_{N \rightarrow +\infty} \sup_{t \in [0, T]} \mathcal{W}_1(\mu(t), \mu^N(t)) = 0.$$

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- Suppose $a \in X$, let $T > 0$ and fix $\mu_0 \in \mathcal{P}_c(\mathbb{R}^d)$.
- Let μ be a weak solution of the c.e. with $\mu(0) = \mu_0$ on $[0, T]$.
- Let $\mu_0^N = \frac{1}{N} \sum_{i=1}^N \delta_{x_{0,i}^N}$ be such that $x_{0,i}^N \sim \mu_0$ i.i.d. $\forall N$ and $\forall i$.

Then, $\exists R > 0$ depending only on T, a , and $\text{supp}(\mu_0)$ such that it holds

$$\text{supp}(\mu^N(t)) \cup \text{supp}(\mu(t)) \subseteq B(0, R), \forall N \in \mathbb{N} \text{ and } \forall t \in [0, T],$$

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The limit functional \mathcal{E}

- Natural candidate for the Γ -limit \mathcal{E} of the \mathcal{E}_N : as μ is the uniform limit of the μ^N then we define

$$\mathcal{E}(\hat{a}) = \frac{1}{T} \int_0^T \int_{\mathbb{R}^d} \left| (F[\hat{a}] - F[a]) * \mu(t) \right|^2 d\mu(t)(x) dt.$$

- Since $\mathcal{E}(\hat{a}) \geq 0$ and $\mathcal{E}(a) = 0$, then a minimizes \mathcal{E} . Is it unique?
- Given $d(x, y) = |x - y|$, introduce the family of measures

$$\varrho(t)(A) = (\mu(t) \otimes \mu(t))(d^{-1}(A)), \text{ for all } t \in [0, T] \text{ and}$$

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- By Jensen or Hölder inequality it holds

$$\mathcal{E}(\hat{a}) \leq \int_{\mathbb{R}_+} |\hat{a}(s) - a(s)|^2 d\rho(s) = \|\hat{a} - a\|_{L_2(\mathbb{R}_+, \rho)}^2$$

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Proposition Fix $M > 0$ and $K = [0, 2R] \subset \mathbb{R}_+$ for some $R > 0$. Then the set

$$X_{M,K} = \{b \in W_\infty^1(K) : \|b\|_{L_\infty(K)} + \|b'\|_{L_\infty(K)} \leq M\}$$

is **relatively compact with respect to the uniform convergence on K** .

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where μ^N is the solution of c.e. with initial datum $\mu_0^N = \frac{1}{N} \sum_{i=1}^N \delta_{x_{0,i}^N}$.
Let $V_N \subset X_{M,K}$ be a sequence with the **uniform approximation property** and consider

$$\hat{a}_N \in \underset{\hat{a} \in V_N}{\operatorname{argmin}} \mathcal{E}_N(\hat{a}).$$

Then $(\hat{a}_N)_{N \in \mathbb{N}}$ **converges uniformly on K** (up to subsequences) to some continuous function $\hat{a} \in X_{M,K}$ such that $\mathcal{E}(\hat{a}) = 0$.

Furthermore...

The Γ -convergence - II

...if the coercivity condition holds, then $\hat{a} = a$ in $L_2(\mathbb{R}_+, \rho)$ and

$$\|\hat{a}_N - a\|_{L_2(\mathbb{R}_+, \rho)} \leq C(M, T, \mu_0)N^{-1}.$$

Proof: by compactness of $X_{M,K}$, the sequence of minimizers $(\hat{a}_N)_{N \in \mathbb{N}}$ admits a subsequence converging to some $\hat{a} \in X_{M,K}$. The uniform approximation property of the V_N implies $\mathcal{E}(b) \geq \mathcal{E}(\hat{a})$ for all $b \in X_{M,K}$, whence $0 = \mathcal{E}(a) \geq \mathcal{E}(\hat{a}) \geq 0$. \square

Problem: the bound M depends on a , but a is unknown!



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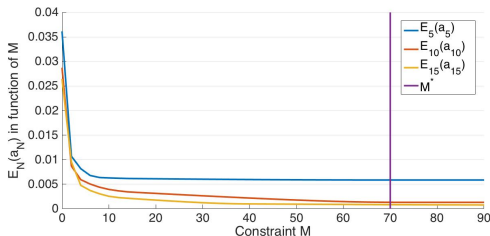
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Solution: For N fixed, $\mathcal{E}_N(\hat{a}_N)$ is decreasing for $M \rightarrow +\infty$ and $\exists M^*$ independent from N such that

$$\frac{\partial \mathcal{E}_N(\hat{a}_N)}{\partial M}(M^*) = 0.$$



Minimizing \mathcal{E}_N is a least squares minimization

The advantage of minimizing $\mathcal{E}_N(\hat{a})$ is that it can be reduced to a simple ℓ_2 minimization. Indeed

- let $V_N = \text{span}\{\varphi_\lambda\}_{\lambda=1}^{D(N)}$ where the φ_λ are a linear B-spline basis with $D(N)$ elements supported on $[0, 2R]$,
- let $0 = t_0 < t_1 < \dots < t_m = T$ be a time discretization,
- let $\dot{x}_i(t_k) = \frac{x_i(t_k) - x_i(t_{k-1})}{t_k - t_{k-1}}$, for every $k \geq 1$ be the finite differences approximating the true velocities,

then the *discrete-time error functional* satisfies

$$\begin{aligned} \bar{\mathcal{E}}_N(\hat{a}) &= \frac{1}{m} \sum_{k=1}^m \frac{1}{N} \sum_{j=1}^N \left| \sum_{\lambda=1}^{D(N)} \frac{a_\lambda}{N} \sum_{i=1}^N \varphi_\lambda(|x_j(t_k) - x_i(t_k)|) (x_j(t_k) - x_i(t_k)) - \dot{x}_i(t_k) \right|^2 \\ &= \frac{1}{mN} \|C\vec{a} - v\|_2^2. \end{aligned}$$

where $\vec{a} = (a_1, \dots, a_{D(N)})$, $v = (\dot{x}_1(t_1), \dots, \dot{x}_N(t_1), \dots, \dot{x}_1(t_m), \dots, \dot{x}_N(t_m))$.



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How we implement the constraints

$$\text{If } D = \begin{bmatrix} 1 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & -1 \\ 0 & 0 & \dots & 0 & 0 \end{bmatrix} \text{ then}$$

$$\|a\|_{L_\infty([0,2R])} \leq 2\|\vec{a}\|_\infty \text{ and } \|a'\|_{L_\infty([0,2R])} \leq \|D\vec{a}\|_\infty,$$

hence we numerically implement the convex constrained minimization

$$\min_{\hat{a} \in V_N} \mathcal{E}_N(\hat{a}) \quad \text{subject to} \quad \|\hat{a}\|_{L_\infty([0,R])} + \|\hat{a}'\|_{L_\infty([0,R])} \leq M,$$

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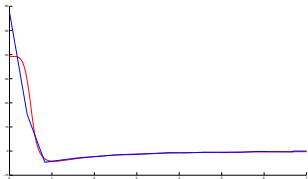
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Varying N - I

d	L	T	M	N	$D(N)$
2	3	0.5	100	[10, 20, 40, 80]	$2N$

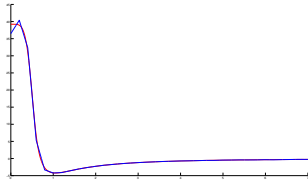
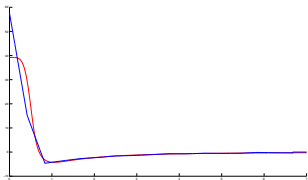
Table: Parameter values



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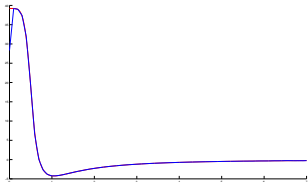
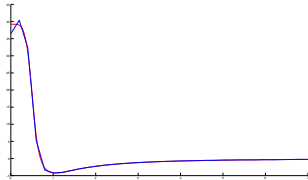
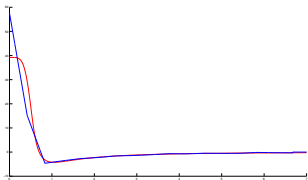
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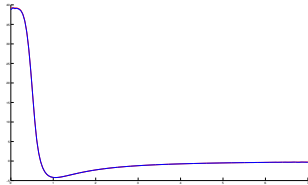
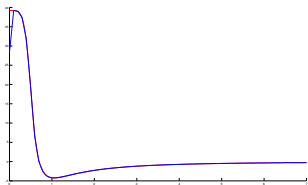
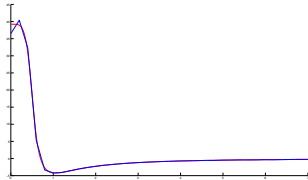
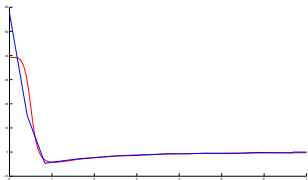
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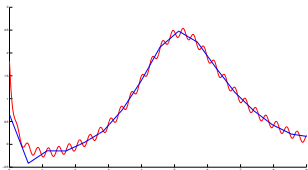
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Varying N - II

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2	3	0.5	100	[10, 20, 40, 80]	$2N$

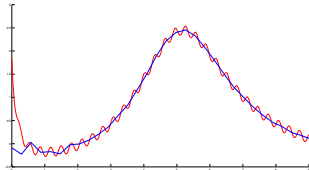
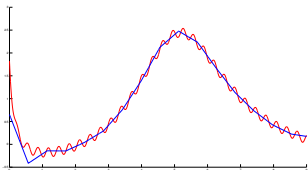
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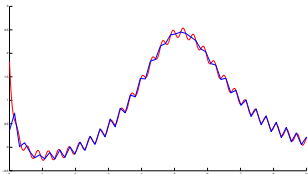
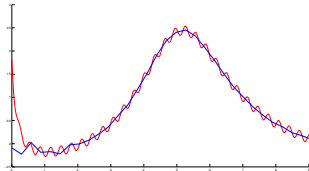
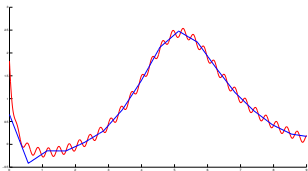
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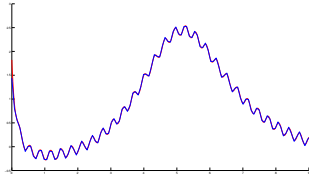
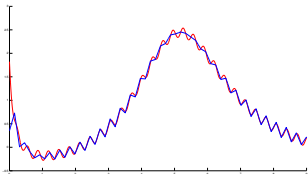
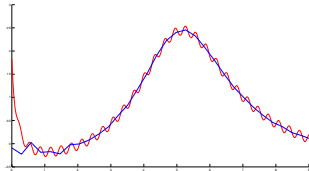
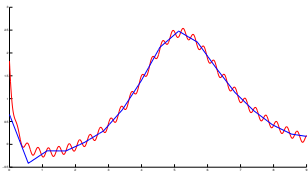
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The coercivity condition

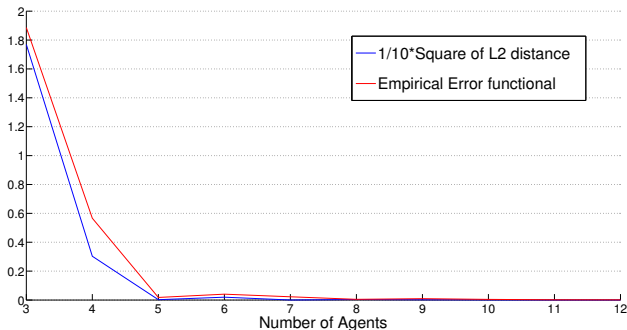


Figure: Plot of $\frac{1}{10} \|a - \hat{a}_N\|_{L_2(\mathbb{R}_+, \rho)}^2$ and $\bar{\mathcal{E}}_N(\hat{a}_N)$. We can estimate the constant c_T with the value $\frac{1}{10}$.

d	T	M	N	$D(N)$
2	0.5	100	[3, 4, ..., 12]	$3N - 5$

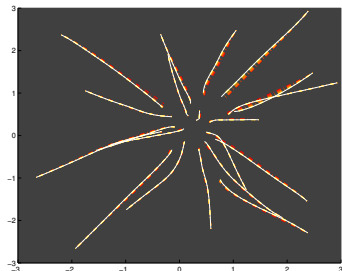
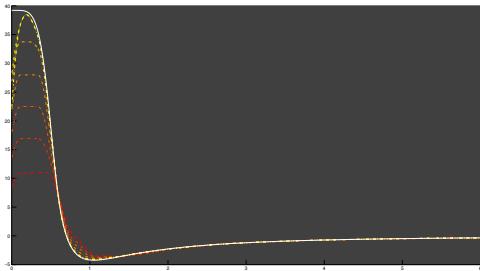
Tuning the constraint M - I

Left: reconstruction of a kernel with different M .

Right: reconstruction of agents' trajectories with different M .

In white: true kernel and true trajectories.

The brighter the reconstruction, the bigger M .



d	L	T	M	N	$D(N)$
2	3	1	$2.7 \times [10, 15, \dots, 40]$	20	60

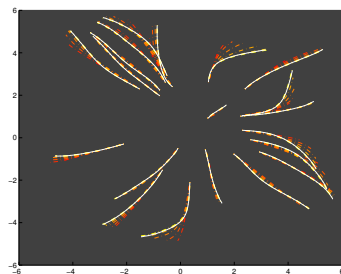
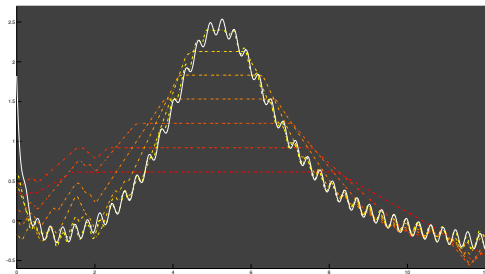
Tuning the constraint M - II

Left: reconstruction of a kernel with different M .

Right: reconstruction of agents' trajectories with different M .

In white: true kernel and true trajectories.

The brighter the reconstruction, the bigger M .



d	L	T	M	N	$D(N)$
2	3	1	$1.25 \times [10, 15, \dots, 40]$	20	150

A few info

- **WWW:** <http://www-m15.ma.tum.de/Allgemeines/MattiaBongini>
- **References:**
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 - G. Albi, M. Bongini, E. Cristiani, D. Kalise, *Invisible Control of Self-Organizing Agents Leaving Unknown Environments*, submitted, 2015.
 - M. Bongini, M. Fornasier, F. Rossi, and F. Solombrino, *Mean-Field Pontryagin Maximum Principle*, submitted, 2015.