Optimization Problems for Interacting Particle Systems and Corresponding Mean-field Limits

René Pinnau¹ and Claudia Totzeck¹

¹ Department of Mathematics, TU Kaiserslautern, 67663 Kaiserslautern

We summarize the relations of optimality systems for an interacting particle dynamic in the microscopic and in the kinetic description. In particular, we answer the question if the passing to the mean-field limit and deriving the first order optimality system can be interchanged without affecting the results. The answer is affirmative, if one derives the optimality system on the kinetic level in the metric space \( (P_2, W_2) \). Moreover, we discuss the relation of to the adjoint PDE derived in the \( L^2 \)-sense. Here, the gradient can be derived as expected from the calculus in Wasserstein space.

© 2019 The Authors Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH Verlag GmbH & Co. KGaA Weinheim

1 Introduction

Interacting particle systems and their kinetic descriptions were extensively studied in the last decades. The applications range from formation of swarms of birds or schools of fish to dogs herding sheep, consensus formation and follower-leader dynamics [1–6]. Recently, even various particle swarm schemes for global optimization were proposed [7, 8]. Follower-leaders or dogs herding a large amount of sheep naturally lead to a kinetic description involving a probability measure representing the positions and velocities of the crowd [9–11]. Naturally, there arises the question of optimal evacuation, leader dynamics or dogs herding sheep, consensus formation, natural leader, and the optimization procedure without affecting the results? The answer is affirmative, if one derives the optimality system on the microscopic level in the metric space \( (P_2, W_2) \) and passing to the mean-field limit and deriving the first order optimality system can be interchanged without affecting the results. The answer is affirmative, if one derives the optimality system on the microscopic level in the metric space \( (P_2, W_2) \) and passing to the mean-field limit following the steps in [14–17] leads to coupled PDE in \( \mathbb{R}^{2d} \) and containing both, state and adjoint information, at once. The high-dimensional PDE is supplemented with both, initial and terminal data. In fact, the initial data is posed in the states and the terminal data for the adjoints. The PDE for the coupled system was found independently in [18, 19] as result of the Pontryagin Principle and the Hamiltonian system corresponding to (Opt).

2 Optimal Control Problem and Relations of the Optimality Systems

We begin with a general problem and restrict the considerations to first order systems. In fact, we consider a fixed time interval \( t \in [0, T] \) and \( N \) interacting particles collected in the vector \( t \mapsto x(t) = (x_i(t))_{i=1,...,N}, x_i(t) \in \mathbb{R}^{dN} \) that encounter some control represented by the variable \( t \mapsto u(t) \in \mathbb{R}^{dm} \). This leads to the general system

\[
\partial_t x = v(x, u), \quad x(0) = x_0.
\]

(P)

Passing to the mean-field limit with the empirical measure \( \mu^N(t, x) = \frac{1}{N} \sum_{i=0}^{N} \delta_0(x - x_i) \), \( N \to \infty \) we obtain the corresponding kinetic formulation

\[
\partial_t \mu + \nabla_x (v(t, x) \mu) = 0.
\]

(MF)

Additionally, we introduce the cost functional which completes the optimization problem

\[
J(x, u) = \int_0^T j(x, t) \, dt + \frac{1}{2} \|u\|_{L^2}^2 \quad \text{subject to} \quad (P) \text{ or } (MF).
\]

(Opt)

The cost functional may for example involve the center of mass or the variance w.r.t \( \mu \). For further details we refer to [10, 12, 13]. The interesting question is now Can we interchange the limit \( N \to \infty \) and the optimization procedure without affecting the results?

The answer is affirmative and the main findings are summarized in the flow chart in Fig. 1. Indeed, starting from the state ODE, one can compute the corresponding adjoint ODE for the adjoint state \( p \) using the standard \( L^2 \)-calculus. Considering now the coupled system of state and adjoint ODEs with its empirical density \( \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i(t), p - p_i(t)) \) and passing to the mean-field limit following the steps in [14–17] leads to coupled PDE in \( \mathbb{R}^{2d} \) and containing both, state and adjoint information, at once. The high-dimensional PDE is supplemented with both, initial and terminal data. In fact, the initial data is posed in the states and the terminal data for the adjoints. The PDE for the coupled system was found independently in [18, 19] as result of the Pontryagin Principle and the Hamiltonian system corresponding to (Opt).
Passing to the limit $N \to \infty$ on the state ODE yields the corresponding state PDE. Further, an adjoint calculus in $(P_2, W_2)$ introduced in [13] leads to a corresponding mean-field adjoint which is an evolution equation for a vector-valued measure. The computations are based on theory discussed in [20–23]. The mean-field adjoint can also be derived from the evolution equation for $\nu$ by taking the first moment w.r.t. the adjoint variable.

On the other hand, one can assume that $\mu$ has an $L^2$-density and apply standard $L^2$-calculus to the state PDE. Then, one obtains a scalar adjoint equation which does not preserve mass. This is expected since the mass-conservation of the transport equation is not included in this metric. Nevertheless, taking the gradient of this adjoint equation and evaluating it along the characteristics of the state ODE leads to the corresponding adjoint particle system. In our opinion, this relation is a justification for using the $L^2$-adjoint, instead of the measure-valued $W$-adjoint, for the numerical treatment of the optimization problem as in [10]. The results therein show that this approach leads to very satisfying results. The relation involving the gradient was found in many other contributions, see for example [24,25]. Another interesting fact is that the $W$-adjoint can be characterized as first moment of the evolution equation for $\nu$. See [13] for more details.

To summarize, passing to the mean-field limit and optimizing can be interchanged, if $(P_2, W_2)$ is chosen as metric space on the PDE level. Moreover, a convergence rate for the convergence of the controls in the limit $N \to \infty$ can be shown [13]. Recent results can be also found in [26].

**References**

[1] J. A. Carrillo, M. Fornasier, G. Toscani, and F. Vecil, Particle, kinetic, and hydrodynamic models of swarming, in: Mathematical Modeling of Collective Behavior in Socio-Economic and Life Sciences, edited by G. Naldi, L. Pareschi, and G. Toscani (Birkhäuser Boston, 2010), pp. 297–336.

[2] S. Roy, M. Annunziato, and A. Borzì, J. Comp. Theo. Transp. (2016).

[3] R. Bailo, M. Bongini, J. Carrillo, and D. Kalise, IFAC-PapersOnLine 51(13), 1–6 (2018).

[4] G. Albi and D. Kalise, IFAC-PapersOnLine 51(3), 86–91 (2018).

[5] N. Bellomo and C. Dogbe, SIAM review 53(3), 409–463 (2011).

[6] G. Naldi, L. Pareschi, and G. Toscani, Mathematical modeling of collective behavior in socio-economic and life sciences (Springer Science & Business Media, 2010).

[7] R. Pinnau, C. Totzeck, O. Tse, and S. Martin, M3AS 27(1) (2017).

[8] J. A. Carrillo, Y. P. Choi, C. Totzeck, and O. Tse, M3AS 28(6), 1037–1066 (2018).

[9] J. A. Carrillo, Y. Choi, and M. Hauray, CISM Volume 553, pp. 1–46 (2014).

[10] M. Burger, R. Pinnau, A. Roth, C. Totzeck, and O. Tse, preprint: arXiv:1903.12407 (2019).

[11] S. Roy, M. Annunziato, A. Borzì, and C. Klingenberg, Computational Optimization and Applications 69(2), 423–459 (2018).

[12] C. Totzeck, Asymptotic Analysis of Optimal Control Problems and Global Optimization (PhD Thesis, TU Kaiserslautern, Verlag Dr. Hut, 2017).

[13] M. Burger, R. Pinnau, C. Totzeck, and O. Tse, preprint: arXiv:1902.05339 (2019).

[14] W. Braun and K. Hepp, Communications in Mathematical Physics (1977).

[15] H. Neunzert, Lecture Notes in Mathematics pp. 60–110 (1984).

[16] R. L. Dobrushin, Functional Analysis and Its Applications 13(2), 115–123 (1979).

[17] F. Golse, Journees Equations aux derivees partielles (2003).

[18] M. Fornasier and F. Solombrino, ESAIM: Control, Optimization, and Calculus of Variations 20(4), 1123–1152 (2014).

[19] M. Bongini, M. Fornasier, F. Rossi, and F. Solombrino, Journal of Optimization Theory and Applications 175(1), 1–38 (2017).

[20] C. Villani, Optimal Transport Old and New (Springer-Verlag B. Hd., Grundlehren der mathematischen Wissenschaften, 2009).

[21] L. Ambrosio, N. Gigli, and G. Savaré, Gradient flows: in metric spaces and in the space of probability measures (Springer Science & Business Media, 2008).

[22] F. Otto, Comm. Part. Diff. Equations 26(1–2), 101–174 (2001).

[23] B. Bonnet and F. Rossi, Calculus of Variations and Partial Differential Equations 58(11) (2019).

[24] M. Herty and C. Ringhofer, preprint: https://www.igpm.rwth-aachen.de/forschung/preprints/489 (2019).

[25] G. Albi, Y. P. Choi, M. Fornasier, and D. Kalise, Applied Mathematics & Optimization 76(1), 93–135 (2017).

[26] M. Fornasier, S. Lisini, C. Orrieri, and G. Savaré, European Journal of Applied Mathematics p. 1–34.