Numerical Identification of Nonlocal Potentials in Aggregation

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Abstract. Aggregation equations are broadly used to model population dynamics with nonlocal interactions, characterized by a potential in the equation. This paper considers the inverse problem of identifying the potential from a single noisy spatial-temporal process. The identification is challenging in the presence of noise due to the instability of numerical differentiation. We propose a robust model-based technique to identify the potential by minimizing a regularized data fidelity term, and regularization is taken as the total variation and the squared Laplacian. A split Bregman method is used to solve the regularized optimization problem. Our method is robust to noise by utilizing a Successively Denoised Differentiation technique. We consider additional constraints such as compact support and symmetry constraints to enhance the performance further. We also apply this method to identify time-varying potentials and identify the interaction kernel in an agent-based system. Various numerical examples in one and two dimensions are included to verify the effectiveness and robustness of the proposed method.

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1 Introduction

Nonlocal Partial Differential Equations (PDE) are often used to model dynamics with nonlocal interactions. They have wide applications in neuronal networks [7], biological

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aggregation [46] and material science [2]. In neuronal networks, nonlocal PDEs are used to describe the dynamics of excitatory neurons' local activities in the cortex, where the nonlocal term models the connection strength between neurons [7]. In biological aggregation, the population density of fish schools can be modeled by a nonlocal PDE [46], where the nonlocal term describes the long-range attraction and short-range repulsion.

In this paper, we consider the aggregation equation

$$u_t + \nabla \cdot (u\mathbf{p}) = 0, \quad \text{with} \quad \mathbf{p} = -\nabla(\phi * u), \tag{1.1}$$

where ϕ is a potential (also known as the kernel), $\phi * u$ denotes the convolution of ϕ and u. This equation has broad applications in physics and biology. In granular materials, (1.1) is used to characterize the dynamics of kinetic models [9]. In biology, the evolution of swarming can be described by (1.1) in which the potential ϕ represents the long-range attraction, and short-range repulsion between individuals [56]. In particular, the authors in [43] show that starting from an Eulerian description of an attraction-repulsion dynamical system, as the number of individuals goes to infinity, the dynamical system converges to (1.1) which describes the evolution of the mean-field spatial density of the population. In bacterial chemotaxis, the convolution $\phi * u$ represents the concentration of chemoattractant which is emitted by bacteria and used to interact with other individuals [33]. A popular model in the kinetic aspect for this dynamics is the Othmer–Dunbar–Alt system whose hydrodynamic limit is (1.1) [17]. Other applications can be found in particle assembly [29], opinion dynamics [44] and pattern formation [1].

Although (1.1) has been successfully applied to model dynamics in different fields, its solution may blow up in the evolution process. It has been shown that, even with a smooth initial condition, when the potential has a Lipschitz point at the origin, a weak solution of (1.1) may always concentrate and become a Dirac function in a finite time, which is known as the finite-time blow-up solution [5]. Here, the potential having a Lipschitz point means that the potential is Lipschitz but has a singular point. This finite-time blow-up behavior of solutions brings difficulties in solving (1.1) numerically, especially near the blow-up time. In [31], the authors use a characteristic method to solve an equivalent coupled ODE system with potential $\phi = |x|$ in various dimensions. The particle method is studied in [13] which enables one to track the behavior of solutions after the blow-up time.

In literature, most existing works focus on the mathematical theories on the existence and regularity of the solution, or the numerical solvers of (1.1) with a given potential. The inverse problem of identifying the potential from a given solution has not been widely studied in comparison with the forward problem. The identification of the potential from the steady-state solution is considered in [22], where finding the underlying potential amounts to solving a time-independent nonlocal PDE. In [58, 59], the authors consider learning the potential in a non-local linear PDE from high-fidelity data. The potential is represented as a linear combination of Bernstein polynomials, and the polynomial coefficients are recovered from an optimization problem solved by the Adam optimizer and L-BFGS. In [6, 41], a variational method is introduced to estimate the kernel from