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 aggrega-
tion, 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

\[ u_t + \nabla \cdot (u \mathbf{p}) = 0, \quad \text{with} \quad \mathbf{p} = -\nabla (\phi \ast u), \]

(1.1)

where \( \phi \) is a potential (also known as the kernel), \( \phi \ast u \) denotes the convolution of \( \phi \) 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 \( \phi \) 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 \( \phi \ast u \) represents the concentration of chemoo-
tractant 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 sys-
tem 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,
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 Lip-
schitz 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 equiv-
alent 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 co-
efficients 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