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Nonlocal diffusion and peridynamic models with Neumann type constraints and their numerical approximations☆

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ABSTRACT

This paper studies nonlocal diffusion models associated with a finite nonlocal horizon parameter δ that characterizes the range of nonlocal interactions. The focus is on the variational formulation associated with Neumann type constraints and its numerical approximations. We establish the well-posedness for some variational problems associated and study their local limit as $\delta \to 0$. A main contribution is to derive a second order convergence to the local limit. We then discuss the numerical approximations including standard finite element methods and quadrature based finite difference methods. We study their convergence in the nonlocal setting and in the local limit.

1. Introduction

Nonlocal diffusion equations and their numerical approximations have been subjects of recent studies. Such models arise in the studies of stochastic jump processes [10,18] and they also share common features with the peridynamic model of continuum mechanics proposed by S. Silling [29]. The latter has been shown to be effective in modeling material singularities [4,8,13,27,31,32] since the model avoids the explicit use of spatial derivatives. Nonlocal models such as peridynamics are often parametrized by a parameter δ that is called the horizon measuring the range of nonlocal interactions.

A feature of nonlocal models, different from the local PDEs, is the treatment of interfaces and domain boundaries. Unlike local boundary conditions, the nonlocal analog may be attributed to how the law of nonlocal interactions gets modified in the presence of physical boundary. Discussions on a variety of nonlocal constraints has been given in [17]. It is known that Neumann type problems presents substantial differences from that on Dirichlet type problems for nonlocal equations, see [2,3,5,6,12,14,17,25,37] for various studies devoted to nonlocal Neumann type problems. Our study here provides new understanding to the proper formulation of Neumann conditions. In particular, we demonstrate how a suitable formulation leads to the second order convergence of the nonlocal models to their local limit in the horizon parameter δ as $\delta \to 0$. Such results are new and are expected to be of optimal order while previous studies have provided at most linear (first order) convergence [19]. Neumann problems are not only interesting on their own but also play important roles in interface problems, free boundary problems, the coupling and domain decomposition of nonlocal problems.

Parallel to the derivation of Neumann problems and their mathematical analysis, it is natural to consider their numerical approximations. For nonlocal models characterized by the parameter δ, it has been known in the literature that as

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$\delta \to 0$, one often encounter consistency issues at both continuum and discrete levels between the nonlocal models and the local PDEs, when the latter remain valid. On the continuum level, the consistency has been established either formally using Taylor expansions of sufficiently smooth solutions [29,30], or more rigorously via functional analytic means without extra regularity assumptions [23,25,34]. With the increasing interests in developing efficient codes for nonlocal models, it is often asked if numerical schemes developed for nonlocal models would produce results consistent with that produced by the local limit models when the horizon is small and with sufficient numerical resolution. Answering such questions on the discrete level is an important task of code validation and verification. In [34], a theory of asymptotically compatible schemes was developed. It was successfully applied to nonlocal models with Dirichlet type nonlocal volumetric constraints. Given the extra complications involved in the nonlocal Neumann type problems, a separate study of similar issues in the Neumann setting is worthwhile. Hence, another contribution of this paper is to demonstrate the applicability of the theory on asymptotically compatible scheme for Neumann type problems.

To highlight the main issues addressed in this manuscript, we summarize several different limiting processes that are of our particularly concern, namely: (1) limit of nonlocal continuum models as the horizon $\delta \to 0$; (2) limit of discrete schemes for nonlocal models as $\delta \to 0$ for a fixed mesh parameter h; (3) limit of discrete schemes of nonlocal models as $h \to 0$ for fixed δ; (4) limit of the discrete schemes for the nonlocal models with both $\delta \to 0$ and $h \to 0$. We present findings on these processes in this work. A one-dimensional model is used for the simplicity in presentation. Our results offer a rigorous mathematical theory behind the nonlocal Neumann type problems and an optimal order error bound between the solutions of nonlocal models and their local limit. They also demonstrate the general applicability of the framework on asymptotically compatible scheme to the numerical discretization of Neumann type problems.

The paper is organized as follows. In Section 2, we introduce the nonlocal Neumann type constrained value problems associated to nonlocal variational problems. The well-posedness of the variational problem is given. A number of key results are stated in Section 3, we analyze the asymptotic compatibility of our nonlocal model. The convergence of nonlocal models to linear local problems is established. Furthermore, we formally estimate the convergence rate as the interaction horizon tends to zero, which is new with regards to previous works. Discussion on the inhomogeneous Neumann type constraints is also made. In Section 4, we present both quadrature based finite difference and finite element discretization schemes. In Section 5, we first discuss how to numerically impose the Neumann constraints and then give related numerical results to further substantiate our theoretical studies. Different limiting processes are examined numerically in this section. Finally, we give some conclusions and remarks in Section 6.

2. Nonlocal variational problems

In this section, we first introduce a nonlocal variational problem with Neumann type volume constraints, along with the associated nonlocal operators and the class of nonlocal interactions kernel to be focused on in this paper. Later, in Sections 2.3 and 2.5, the natural energy space and the well-posedness of nonlocal problems are studied. The studies here are parallel to the traditional analysis of local second order elliptic equations as well as the analysis of nonlocal diffusion models with Dirichlet type constraints, but with necessary modifications. We refer to [17] for more discussions on the differences and connections between local and nonlocal steady-state diffusion problems.

2.1. Nonlocal variational problems

Let $\Omega \subset \mathbb{R}^d$ denote a bounded, open domain with a piecewise planar boundary. Consider the nonlocal energy functional

$$E(u) = \frac{1}{2}\int_\Omega\int_\Omega \rho_\delta(\mathbf{x}', \mathbf{x})\big(u(\mathbf{x}') - u(\mathbf{x})\big)^2 d\mathbf{x}' d\mathbf{x}, \tag{1}$$

where $\rho_\delta(\mathbf{x}', \mathbf{x}) = \rho_\delta(\mathbf{x}, \mathbf{x}')$ is a symmetric, nonnegative interaction kernel with the property that $\rho_\delta(\mathbf{x}', \mathbf{x}) = 0$ if $|\mathbf{x}' - \mathbf{x}| > \delta$. Here $|\mathbf{x}' - \mathbf{x}|$ denotes the distance between $\mathbf{x}'$ and $\mathbf{x}$.

Without loss of generality, for given data $f = f(\mathbf{x})$ defined on Ω, with the total net-flux assumed to be zero, the following compatibility condition is assumed:

$$\int_\Omega f(\mathbf{x}) d\mathbf{x} = 0\,. \tag{2}$$

This type of compatibility is also present in Neumann type problems associated with local elliptic operators. We then define the total energy

$$E_f(u) = \frac{1}{2}\int_\Omega\int_\Omega \rho_\delta(\mathbf{x}', \mathbf{x})\big(u(\mathbf{x}') - u(\mathbf{x})\big)^2 d\mathbf{x}' d\mathbf{x} - \int_\Omega f(\mathbf{x}) u(\mathbf{x}) d\mathbf{x}\,. \tag{3}$$

2.2. Nonlocal kernel

We assume that the symmetric, non-negative kernel ρ satisfies, for all $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$,

$$\rho_\delta(\mathbf{x}', \mathbf{x}) = \begin{cases} \rho_\delta(|\mathbf{x}' - \mathbf{x}|) \ge 0, & \text{if } |\mathbf{x}' - \mathbf{x}| \le \delta, \\ 0, & \text{if } |\mathbf{x}' - \mathbf{x}| > \delta, \end{cases} \tag{4}$$

and

$$\int_{\mathbb{R}^d} \rho_\delta(\mathbf{x},\mathbf{x}')|\mathbf{x}'-\mathbf{x}|^2 d\mathbf{x}' = \int_{|\mathbf{x}'-\mathbf{x}|\le\delta} \rho_\delta(\mathbf{x},\mathbf{x}')|\mathbf{x}'-\mathbf{x}|^2 d\mathbf{x}' = 1. \tag{5}$$

We note that, in this work, the normalization is taken over $\mathbb{R}^d$ and independent of the domain Ω. Other formulations such as heterogeneously defined or position aware horizons [26,35] are beyond the scope of the current work and will be examined in the future. We will have more detailed discussions on the assumption (5) in later sections. A popular case to study is given by

$$\rho_\delta(\mathbf{x},\mathbf{x}') = \frac{c}{\delta^{d+2}}\gamma\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\delta}\right) \text{ for all } \mathbf{x},\mathbf{x}' \in \mathbb{R}^d, \tag{6}$$

with γ being a non-increasing function having compact support in a unit ball. Here c is the scaler to make ρ_δ satisfy condition (5). We will not attempt to make the study applicable to the most general kernels.

2.3. Function space

The space of interest to us, denoted by $\mathcal{S}(\Omega)$, is a subspace of $L^2(\Omega)$ given by

$$\mathcal{S}(\Omega) = \left\{u \in L^2(\Omega) : \int_\Omega\int_\Omega \rho_\delta(\mathbf{x},\mathbf{x}')|u(\mathbf{x}')-u(\mathbf{x})|^2 d\mathbf{x}' d\mathbf{x} < \infty\right\}.$$

$\mathcal{S}(\Omega)$ is often called the nonlocal energy space. Furthermore, with the compatibility condition (2), the nonlocal constrained energy space is defined by

$$\mathcal{S}_\delta(\Omega) = \left\{u \in \mathcal{S}(\Omega) : \int_\Omega u d\mathbf{x} = 0\right\}.$$

which is a real inner product space with the inner product $(\cdot,\cdot)_s$ defined as

$$(u,w)_s = B_\delta(u,w).$$

We use $\|u\|_s$ to denote the induced norm $\sqrt{(B_\delta(u,u))}$ of u in $\mathcal{S}_\delta(\Omega)$. For $\{\mathcal{S}_\delta\}$ defined earlier, $\|\cdot\|_s$ is equivalent to a full norm, as demonstrated by the Poincaré inequality given later. Following the same argument as in [23], it can be established that, for any nonnegative, radial kernel with a constant horizon δ, the constrained energy space $\mathcal{S}_\delta(\Omega)$ is a Hilbert space with the norm $\|\cdot\|_s$.

2.4. The variational problem

Consider the constrained minimization problem

$$\min_{u\in\mathcal{S}(\Omega)} E_f(u) \quad \text{subject to} \quad E_c(u) = 0,$$

where $E_c = E_c(u)$ denotes a constraint functional. For example, let

$$E_c(u) := \int_\Omega u(\mathbf{x})\, d\mathbf{x} = 0\,. \tag{7}$$

We then have the equivalent formulation as $\min_{u\in\mathcal{S}_\delta(\Omega)} E_f(u)$.

With the compatibility condition (2), the Euler–Lagrange equations for (3) becomes

$$B_\delta(u,v) = \int_\Omega\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})\big(u(\mathbf{x}')-u(\mathbf{x})\big)\big(v(\mathbf{x}')-v(\mathbf{x})\big) d\mathbf{x}' d\mathbf{x} = (f,v) \tag{8}$$

where

$$(f,v) = \int_\Omega f(\mathbf{x})v(\mathbf{x})d\mathbf{x}$$

and $B_\delta(\cdot,\cdot)$ defines a symmetric bilinear form. The Lagrange multiplier for the constraint on u vanishes for compatible f. Thus, by defining the nonlocal operator

$$u \mapsto \mathcal{L}_\delta u := -2\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})\big(u(\mathbf{x}')-u(\mathbf{x})\big)d\mathbf{x}', \tag{9}$$

we end up with a nonlocal integral equation

$$\begin{cases} \mathcal{L}_\delta u = f & \text{in } \Omega\,, \\ \int_\Omega u = 0 \end{cases} \tag{10}$$

for data f satisfying

$$\int_\Omega f(\mathbf{x})d\mathbf{x} = 0\,.$$

One can see that the compatibility condition on f is a consequence of the anti-symmetry of $\rho_\delta(\mathbf{x}',\mathbf{x})(u(\mathbf{x}')-u(\mathbf{x}))$ in $\mathbf{x}$ and $\mathbf{x}'$ so that

$$\int_\Omega f(\mathbf{x})d\mathbf{x} = \int_\Omega \mathcal{L}_\delta u(\mathbf{x})d\mathbf{x} = -2\int_\Omega\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})\big(u(\mathbf{x}')-u(\mathbf{x})\big)d\mathbf{x}'d\mathbf{x} = 0\,.$$

We note that the difference between the above problem (10) with those corresponding to the Dirichlet type volumetric constraints is that no values of the solution u is specified in any subdomain of Ω, this is consistent to the nature of Neumann conditions which are natural conditions implied by the variational principle. Moreover, for nonlocal models, the information of the Neumann type conditions is encoded in the equations themselves, see [15,16] for detailed accounts on how one may symbolically rewrite (10) as a combination of balance laws in a subset of Ω and a (nonlocal) flux condition in its complement.

We also note that the operator $\mathcal{L}_\delta$ can be written as $\mathcal{L}_\delta = -\mathcal{D}\rho_\delta\mathcal{D}^*$ where $\mathcal{D}$ and $\mathcal{D}^*$ are the basic nonlocal divergence operator and its adjoint defined in a nonlocal vector calculus given in [16]. Such a formulation draws the natural analogy between nonlocal operators and local second order elliptic differential operators (or more specifically, second order derivative operators in our current setting).

2.5. Well-posedness of nonlocal Neumann problems

Well-posedness of nonlocal Neumann volume-constrained problems has been shown in many previous studies with some conditions imposed on the kernel. see for instance [3,5,6,15,23] and the references cited therein. For completeness, we include a brief discussion on Neumann type problems here. The study utilizes extensions of the ideas in [9], see also [1,21,22,24,25,28] for additional discussions. A key is the following nonlocal Poincaré-type inequality that holds over all subspaces of functions in $L^2(\Omega)$ satisfying certain compatible constraints. We begin with Proposition 1 of [23].

Proposition 2.1. *[25, Proposition 1] Suppose that ρ_δ satisfies (4), (5) and V is a closed subspace of $L^2(\Omega)$ that intersects $\mathbb{R}^d$ trivially. Then there exists $C = C(\rho_\delta, V, \Omega)$ such that*

$$\|u\|^2 \le C\int_\Omega\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})|\mathbf{x}'-\mathbf{x}|^2(u(\mathbf{x}')-u(\mathbf{x}))^2 d\mathbf{x}'d\mathbf{x}\,,\quad \forall u\in V. \tag{11}$$

A strengthened nonlocal Poincaré inequality is given later with a sharper constant C independent of the horizon δ. A consequence of the nonlocal Poincaré-type inequality is the coercivity of the bilinear form $B = B_\delta(u,v)$. A standard application of Lax–Milgram theory or Riesz representation theorem then yields the well-posedness of the variational problem.

Proposition 2.2. *Suppose that ρ_δ satisfies (4), (5) and V is a closed subspace of $L^2(\Omega)$ that intersects $\mathbb{R}^d$ trivially. Then there exists $\kappa = \kappa(\rho_\delta, V, \Omega)$ such that*

$$\|u\|_s^2 \le \kappa B_\delta(u,u),\quad \text{for all} u\in V\cap\mathcal{S}(\Omega).$$

Consequently, for a given $f\in L^2$ satisfying (2), by taking $\mathcal{V} = \mathcal{S}_\delta(\Omega)$, we see that there exists a unique $u\in\mathcal{S}_\delta(\Omega)$ such that

$$B_\delta(u,v) = (f,v),\quad \forall v\in\mathcal{S}_\delta(\Omega). \tag{12}$$

Moreover, $|u|_s = |f|_{\mathcal{S}_\delta^*(\Omega)}$ where $\mathcal{S}_\delta^*(\Omega)$ denote the dual space of $\mathcal{S}_\delta(\Omega)$.

It follows then that the operator $\mathcal{L}_\delta$ restricted on $\mathcal{S}_\delta(\Omega)$, that is, $\mathcal{L}_\delta : \mathcal{S}_\delta(\Omega) \to \mathcal{S}_\delta^*(\Omega)$ is an isometry. In addition, the restriction of the inverse operator $\mathcal{L}_\delta^{-1}$ to $L^2(\Omega)$, that is, $\mathcal{L}_\delta^{-1} : L^2(\Omega) \to \mathcal{S}_\delta(\Omega)$ and satisfies the inequality $|\mathcal{L}_\delta^{-1}f|_s \le C\|f\|_{L^2}$. This follows from the continuous embedding of $L^2(\Omega)$ into $\mathcal{S}_\delta^*(\Omega)$ and $\|f\|_{\mathcal{S}_\delta^*(\Omega)} \le \|f\|_{L^2(\Omega)}$ for any $f\in L^2(\Omega)$.

3. The local limit with vanishing horizon

Although we are interested in studying nonlocal models, it is important to get consistency with classical local models when the latter are valid and applicable. For suitably defined kernels, limiting local models of nonlocal models are indeed well-defined. While there have been existing studies on similar limiting process for Dirichlet type volume constraints, the case for Neumann type problem presents some different issues.

For a point $\mathbf{x}\in\Omega_\delta = \{\mathbf{x}\in\Omega \mid \text{dist}(\mathbf{x},\partial\Omega) > \delta\}$, we know that

$$\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})(\mathbf{x}'-\mathbf{x})d\mathbf{x}' = 0\,, \tag{13}$$

and

$$\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})|\mathbf{x}'-\mathbf{x}|^2 d\mathbf{x}' = 1\,,\quad \int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})(\mathbf{x}'-\mathbf{x})^k d\mathbf{x}' = o(1)\quad \forall k>2\,. \tag{14}$$

With these assumptions, for any smooth enough function u we have formally that $\mathcal{L}_\delta$ represents a nonlocal diffusion operator with a local limit

$$\mathcal{L}_\delta u(\mathbf{x}) \to \mathcal{L}_0 u(\mathbf{x}) := -\Delta u(\mathbf{x})$$

for $\mathbf{x} \in \Omega_\delta$, which is a fact widely stated in many earlier studies. What concerns us is, when taking into account the modifications in the layer around the boundary of Ω, the formal order of convergence rate as $\delta \to 0$.

To better illustrate our idea, we let Ω be a finite bar in $\mathbb{R}$. Without loss of generality, we can let $\Omega = (0, 1)$. Given data $f = f(x)$, we introduce a modified body force

$$f_\delta(x) = f(x) - \frac{1}{2}\left(\int_\Omega \rho_\delta(x+y)(y^2-x^2)(f(x)+f(y))dy + \int_\Omega \rho_\delta(x+y-2)(x+y-2)(y-x)(f(x)+f(y))dy\right). \tag{15}$$

It is simple to check that:

Lemma 3.1. *The modified function f_δ satisfies the compatibility condition (2) and $f_\delta(x) = f(x)$ for $x \in \Omega_\delta$.*

Instead of (10), we consider the following nonlocal equation

$$\begin{cases} \mathcal{L}_\delta u = f_\delta & \text{on } \Omega\,, \\ \int_\Omega u = 0\,. \end{cases} \tag{16}$$

The limiting local model of (16) is given by

$$\begin{cases} \mathcal{L}_0 u = f & \text{in } \Omega\,, \quad u'(0) = u'(1) = 0\,, \\ \int_\Omega u(x)dx = 0\,. \end{cases} \tag{17}$$

Let

$$\mathcal{S}_0 = \{u \in H^1(\Omega) : \int_\Omega u(x)dx = 0\}$$

with an inner product and norm

$$(u, v)_{\mathcal{S}_0} = \int_\Omega u'(x)v'(x)dx, \quad \|u\|_{\mathcal{S}_0} = \left(\int_\Omega |u'(x)|^2 dx\right)^{\frac{1}{2}},$$

and a bilinear form

$$B_0(u, v) = (u, v)_{\mathcal{S}_0} = \int_\Omega u'(x)v'(x)dx\,, \tag{18}$$

for $u, v \in \mathcal{S}_0$. The weak formulation of (17) can be cast in the same form as (12) with $\delta = 0$.

3.1. Convergence of variational solutions

To study the asymptotic property of the nonlocal model as $\delta \to 0$, we need a “sharper” version of Poincaré inequality, that is, the Poincaré constant in the inequality should be independent of the horizon δ. This can be worked out, for instance, by following [24] to consider a sequence of radial kernels $\rho_n (n \geq 1)$ satisfying:

$$\xi^{-2}\rho_n(\xi) \text{ is nonnegative and nonincreasing in } |\xi|, \tag{19}$$

$$\int_{\mathbb{R}} \rho_n(|\xi|)d\xi = 1, \tag{20}$$

$$\text{and } \lim_{n\to\infty} \int_{|\xi|\geq r} \rho_n(|\xi|)d\xi = 0, \quad \forall r > 0. \tag{21}$$

Note that in our case, if we let $\rho_\delta(|\xi|) = \xi^{-2}\rho_n(|\xi|)$ and $\delta = \frac{1}{n}$, then the kernel satisfies all the assumptions above. So we have the following variant of the Poincaré-type inequality

Lemma 3.2. *[26, Lemma 4.1] There exists $C > 1$ and $\delta_0 \leq 1$ such that*

$$\|u\|^2 \leq C\int_\Omega\int_\Omega \rho_\delta(x', x)(u(x') - u(x))^2 dx'dx \tag{22}$$

for all $u \in \mathcal{S}_\delta$ and all $\delta \leq \delta_0$.

From the lemma, we can get that

$$\|u\|^2 \leq CB_\delta(u, u)$$

with the same constant C for all $u \in \mathcal{S}_\delta$, independent of δ. The uniform boundedness of $\mathcal{L}_\delta^{-1}$ in L^2 norm then follows from the uniform Poincaré inequality (Theorem 3.2).

Theorem 3.3. *There exists a constant C which is independent of the horizon δ such that*

$$\|\mathcal{L}_\delta^{-1}\|_{L^2} \le C,$$

To study the limiting behavior of the nonlocal solution, we also need a compactness lemma that can be found in [24].

Lemma 3.4. *Suppose* $u_n \in \mathcal{S}_{\delta_n}$ *with* $\delta_n \to 0$. *If*

$$\sup_n \int_\Omega \int_\Omega \rho_{\delta_n}(x', x)(u_n(x') - u_n(x))^2 dx' dx \le \infty,$$

then u_n *is precompact in* $L^2(\Omega)$. *Moreover, any limit point* $u \in \mathcal{S}_0$.

Now we state some convergence results for the solutions of the parametrized variational problems as $\delta \to 0$. We consider the original problem (10) first and the same result for (16) with data f_δ is given in the subsequent Corollary.

Theorem 3.5. *Suppose* u_δ *is the weak solution of (10) and* u_0 *is the weak solution of (17). Then we have*

$$\|u_\delta - u_0\|_{L^2} \to 0 \quad \text{as } \delta \to 0.$$

Proof. Since $B_\delta(u_\delta, v) = (f, v)_{L^2}$ for any $v \in \mathcal{S}_\delta$, by Lemma 22 and uniform Poincaré inequality, for some constants C_1 and C_2 we have

$$C_1\|u_\delta\|_{\mathcal{S}_\delta}^2 \le B_\delta(u_\delta, u_\delta) = (f, u_\delta)_{L^2} \le \|f\|_{L^2}\|u_\delta\|_{L^2} \le C_2\|f\|_{L^2}\|u_\delta\|_{\mathcal{S}_\delta},$$

which leads to the uniform boundedness of $\{u_\delta \in \mathcal{S}_\delta\}$. Thus by the asymptotically compact embedding property, we get the convergence of a subsequence of $\{u_\delta\}$ in L^2 to a limit point $u_* \in \mathcal{S}_0$. For notational convenience, we use the same $\{u_\delta\}$ to denote the subsequence. We claim that

$$B_0(u_*, v) = (f, v)_{L^2}, \quad \forall v \in C^\infty(\Omega).$$

Moreover, since $C^\infty(\Omega)$ is dense in $H^1(\Omega)$, we see that u_* is the unique weak solution u_0 of (17) and the convergence of the whole sequence also follows.

Indeed, let ϕ_ϵ be standard mollifiers so

$$\int_{B(0,\epsilon)} \phi_\epsilon(x) dx = 1\,.$$

Let

$$u_{\delta,\epsilon} = u_\delta * \phi_\epsilon = \int_{B(0,\epsilon)} u_\delta(x-y)\phi_\epsilon(y) dy\,.$$

Define $\Omega_\epsilon = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) > \epsilon\}$. Then for all $v \in C^\infty(\Omega)$,

$$\begin{aligned}&\int_{\Omega_\epsilon}\int_{\Omega_\epsilon} \rho_\delta(x, x')(u_{\delta,\epsilon}(x') - u_{\delta,\epsilon}(x))(v(x') - v(x)) dx' dx \\ &= \int_{B(0,\epsilon)} \phi_\epsilon(y)\left(\int_{\Omega_\epsilon}\int_{\Omega_\epsilon} \rho_\delta(x, x')(u_\delta(x'-y) - u_\delta(x-y))(v(x') - v(x)) dx' dx\right) dy.\end{aligned}$$

Denote

$$B_\delta^\epsilon(u, v) = \int_{\Omega_\epsilon}\int_{\Omega_\epsilon} \rho_\delta(x, x')(u(x') - u(x))(v(x') - v(x)) dx' dx\,,$$

$$B_0^\epsilon(u, v) = \int_{\Omega_\epsilon} u'(x) v'(x) dx$$

and $u_\delta^y(x) = u_\delta(x-y)$, we have

$$B_\delta^\epsilon(u_{\delta,\epsilon}, v) = \int_{B(0,\epsilon)} \phi_\epsilon(y) B_\delta^\epsilon(u_\delta^{\mathbf{y}}, v) dy. \tag{23}$$

We want to show that by letting $\delta \to 0$ first and then letting $\epsilon \to 0$, the left hand side of (23) goes to $B_0(u_*, v)$ and the right hand side goes to $(f, v)_{L^2}$.

Consider the left hand side of (23), for fixed ϵ and small enough δ, $\Omega_\epsilon \subset \Omega_\delta$. Then

$$\begin{aligned}B_\delta^\epsilon(u_{\delta,\epsilon}, v) =& \int_{\Omega_\epsilon}\int_{\Omega} \rho_\delta(x, x')(u_{\delta,\epsilon}(x') - u_{\delta,\epsilon}(x))(v(x') - v(x)) dx' dx \\ &- \int_{\Omega_\epsilon}\int_{\Omega\setminus\Omega_\epsilon} \rho_\delta(x, x')(u_{\delta,\epsilon}(x') - (x))(v(x') - v(x)) dx' dx.\end{aligned}$$

For the first term, by the fact $u_{\delta,\epsilon} \to u_{*,\epsilon}$ in $C^\infty(\Omega)$ and Dominated Convergence Theorem, we have

$$\lim_{\epsilon\to 0}\lim_{\delta\to 0}\int_{\Omega_\epsilon}\int_{\Omega}\rho_\delta(x,x')(u_{\delta,\epsilon}(x')-u_{\delta,\epsilon}(x))(v(x')-v(x))dx'dx = \lim_{\epsilon\to 0} B_0^\epsilon(u_{*,\epsilon},v) = B_0(u_*,v).$$

For the second term, since the integrand is uniformly bounded, we have

$$\lim_{\epsilon\to 0}\lim_{\delta\to 0}\Big|\int_{\Omega_\epsilon}\int_{\Omega\setminus\Omega_\epsilon}\rho_\delta(x,x')(u_{\delta,\epsilon}(x')-u_{\delta,\epsilon}(x))(v(x')-v(x))dx'dx\Big|$$
$$\le C\lim_{\epsilon\to 0}|\Omega_\epsilon||\Omega\setminus\Omega_\epsilon| = 0.$$

Thus we have

$$B_\delta^\epsilon(u_{\delta,\epsilon},v)\to B_0(u_*,v).$$

For the right hand side of (23), define

$$\Delta_\epsilon = |B_\delta^\epsilon(u_\delta^y,v)-B_\delta(u_\delta,v)|.$$

Since $B_\delta(u_\delta,v)=(f,v)_{L^2}$ for all smooth v, it suffices to show that Δ_ϵ is bounded by some constant which is independent of δ and $\Delta_\epsilon\to 0$ as $\epsilon\to 0$. Now define $\Omega_\epsilon^y=\{x\in\Omega : x-y\in\Omega_\epsilon\}$, since the kernel is translation invariant, i.e. $\rho_\delta(x+y,x'+y)=\rho_\delta(x,x')$ if $x+y$ and $x'+y$ are in Ω, we have

$$\int_{\Omega_\epsilon}\int_{\Omega_\epsilon}\rho_\delta(x,x')(u_\delta(x'-y)-u_\delta(x-y))(v(x')-v(x))dx'dx$$
$$=\int_{\Omega_\epsilon^y}\int_{\Omega_\epsilon^y}\rho_\delta(x,x')(u_\delta(x')-u_\delta(x))(v(x'+y)-v(x+y))dx'dx.$$

Therefore,

$$\Delta_\epsilon \le I + II,$$

where

$$I=\left|\int_{\Omega_\epsilon^y}\int_{\Omega_\epsilon^y}\rho_\delta(x,x')(u_\delta(x')-u_\delta(x))(v(x')-v(x))dx'dx-\int_{\Omega}\int_{\Omega}\rho_\delta(x,x')(u_\delta(x')-u_\delta(x))(v(x')-v(x))dx'dx\right|$$

and

$$II=\left|\int_{\Omega_\epsilon^y}\int_{\Omega_\epsilon^y}\rho_\delta(x,x')(u_\delta(x')-u_\delta(x))(v(x'+y)-v(x')-(v(x+y)-v(x)))dx'dx\right|.$$

Note that

$$I = 2\Big|\int_{\Omega\setminus\Omega_\epsilon^y}\int_\Omega\rho_\delta(x,x')(u_\delta(x')-u_\delta(x))(v(x')-v(x))dx'dx\Big|$$
$$\le 2\|u_\delta\|_{\mathcal{S}_\delta}\left(\int_{\Omega\setminus\Omega_\epsilon^y}\int_\Omega\rho_\delta(x,x')(v(x')-v(x))^2dx'dx\right)^{\frac12}$$
$$\le C\left(\int_{\Omega\setminus\Omega_{2\epsilon}}\int_\Omega\rho_\delta(x,x')(v(x')-v(x))^2dx'dx\right)^{\frac12}.$$

The last inequality holds because of $\Omega_{2\epsilon}\subset\Omega_\epsilon^y$. Since v is also in $\mathcal{S}_\delta$, by Bounded Convergence Theorem, we can get $I\to 0$ as $\epsilon\to 0$.

Consider II, since v is smooth, we have

$$II\le\|u_\delta\|_{\mathcal{S}_\delta}\|v(x+y)-v(x)\|_{\mathcal{S}_\delta(\Omega_\epsilon^y)}\le C\|u_\delta\|_{\mathcal{S}_\delta}\|v(x+y)-v(x)\|_{\mathcal{S}_0(\Omega_\epsilon^y)},$$

which also goes to 0 when $\epsilon\to 0$ since $|y|<\epsilon$. □

Corollary 3.6. *Suppose u_δ is the weak solution of (16) and u_0 is the weak solution of (17). Then we have*

$$\|u_\delta-u_0\|_{L^2}\to 0 \quad \text{as } \delta\to 0\,.$$

Proof. Let us assume that $\tilde{u_\delta}$ is the weak solution of (10). By the theorem stated above, it suffices to show that $\|\tilde{u_\delta}-u_\delta\|_{L^2}\to 0$ as $\delta\to 0$, which can be derived from Theorem 3.3 and the fact that

$$\|f-f_\delta\|_{L^2}\to 0 \quad \text{as } \delta\to 0\,.$$

Indeed, denote by $\phi_\delta(x)=\int_\Omega\rho_\delta(x+y)(y^2-x^2)dy$, then ϕ_δ is compactly supported in $x\in[0,\delta]$ and

$$|\phi_\delta(x)|\le\int_\Omega\rho_\delta(x+y)|y^2-x^2|dy\le\int_\Omega\rho_\delta(x+y)(x+y)^2dy\,,$$

which is bounded for any $x \in [0, \delta]$. Moreover, we also have

$$\int_{\Omega} \rho_\delta(x+y-2)(x+y-2)(y-x)dy = \phi_\delta(1-x)\,,$$

which is compactly supported in $x \in [1-\delta, 1]$ and is also bounded. Therefore, when $x \in [0, \delta]$,

$$|f(x) - f_\delta(x)| \le \frac{|f(x)|}{2}\left|\int_{\Omega} \rho_\delta(x+y)(y^2-x^2)dy\right| + \frac{1}{2}\left|\int_{\Omega} \rho_\delta(x+y)(y^2-x^2)f(y)dy\right|.$$

The first integral is bounded and by Schwarz's inequality,

$$\begin{aligned}\left|\int_{\Omega} \rho_\delta(x+y)(y^2-x^2)f(y)dy\right|^2 &\le \int_{\Omega} \rho_\delta(x+y)(y-x)^2dy\int_{\Omega} \rho_\delta(x+y)(x+y)^2f(y)^2dy\\ &\le \int_{\Omega} \rho_\delta(x+y)(x+y)^2dy\int_{\Omega} f(y)^2dy\\ &\le \|f\|_{L^2}\,.\end{aligned}$$

Then we can get that

$$\|f - f_\delta\|_{L^2[0,\delta]} \le C_1\|f\|_{L^2[0,\delta]} + C_2\delta\,,$$

which vanishes as $\delta \to 0$. Similarly, we also have

$$\|f - f_\delta\|_{L^2[1-\delta,1]} \to 0$$

as $\delta \to 0$. Then the claim is true since $f(x) - f_\delta(x) = 0$ for $x \in [\delta, 1-\delta]$. □

The above theorem finally confirms that (17) is the limiting local problem of our nonlocal diffusion problems with Neumann type constraints.

3.2. Order of convergence

Our next aim is to estimate the formal order of convergence rate as $\delta \to 0$, in the presence of Neumann type constraints. Towards this goal, we consider an even more general setting by imposing a mixed type of volume constraints. For simplicity in presentation, we consider the case $\Omega = (0, 1)$ with a Neumann type volume constraint at $x = 0$ and a nonlocal Dirichlet type constraint at $\Omega_D = [1, 1+\delta]$. In this case, the nonlocal operator given by (9) should be properly modified as

$$u \mapsto \mathcal{L}_\delta u := -2\int_{\Omega\cup\Omega_D} \rho_\delta(x', x)\big(u(x') - u(x)\big)dx', \tag{24}$$

Then the nonlocal equation to be solved is

$$\begin{cases}\mathcal{L}_\delta u = f_\delta^L & \text{on } \Omega\,,\\ u = 0 & \text{on } \Omega_D\,,\end{cases} \tag{25}$$

where the one-sided modified body force f_δ^L is given by

$$f_\delta^L(x) = f(x) - \frac{1}{2}\int_{\Omega\cup\Omega_D} \rho_\delta(x+y)(y^2-x^2)(f(x)+f(y))dy$$

for any $x \in \Omega$. The corresponding limiting local model of (25) is given by

$$\begin{cases}\mathcal{L}_0 u = f & \text{in } \Omega\,,\\ u'(0) = 0\,, & u(1) = 0\,.\end{cases} \tag{26}$$

Note that we always choose f such that the exact solution u_0 of the local problem (26) decays smoothly to zero on the Dirichlet side and therefore we can zero extend u_0 to Ω_D smoothly. We first remark that the use of the nonlocal δ-layer (such as $\Omega_D = [1, 1+\delta]$ for the 1-D case) for imposing Dirichlet type of constraints is a feature of nonlocal interaction that has been discussed in many previous works [15]. Effectively, we are now treating $\Omega \cup \Omega_D = [0, 1+\delta]$ as the material body but assuming that $u = 0$ over $[1, 1+\delta]$, the δ neighborhood on the right end, which is a typical feature of nonlocal interaction that has been discussed in many previous works [15]. Due to mixed volume constraints, we have the nonlocal maximum principle stated below.

Lemma 3.7 (Maximum principle)**.** *Let ρ_δ satisfy (13). If $u \in C(\overline{\Omega})$ and $\mathcal{L}_\delta u(x) \le 0$ for all $x \in \Omega$, then*

$$\sup_{x\in\Omega} u(x) \le \sup_{x\in\Omega_D} u(x)\,.$$

Proof. Step 1. We are going to show that the claim is true if $\mathcal{L}_\delta u(x) \le -\epsilon$ for $x \in \Omega$, where $\epsilon > 0$. Assume that $\sup_{x\in\Omega} u(x) > \sup_{x\in\Omega_D} u(x)$. Then since $u \in C(\overline{\Omega})$, we can find $x^* \in \Omega$ such that $u(x^*) = \sup_{x'\in\Omega} u(x') \ge u(x)$ for any $x \in \Omega\cup\Omega_D$. Thus

$$\mathcal{L}_\delta u(x^*) = -\int_{\Omega\cup\Omega_D} \rho_\delta(|x-x'|)(u(x') - u(x^*))dx' \ge 0\,,$$

which contradicts with $\mathcal{L}_\delta u(x) \le 0, \forall x \in \Omega$. So it must be true that $\sup_{x\in\Omega} u(x) \le \sup_{x\in\Omega_D} u(x)$.

Step 2. Now we show that the claim is true if $\mathcal{L}_\delta u(x) \le 0$. Let $w(x) = u(x) + \epsilon x^2$, then one can show that

$$\mathcal{L}_\delta w(x) \le -\epsilon \int_{\Omega\cup\Omega_D} \rho_\delta(|x-x'|)(x'^2 - x^2)dx' \le -\epsilon \,.$$

Therefore, from step 1 we know that for any $\epsilon > 0$

$$\sup_{x\in\Omega} w(x) = \sup_{x\in\Omega} u(x) + \epsilon \le \sup_{x\in\Omega_D} w(x) = \sup_{x\in\Omega_D} u(x) + \epsilon(1+\delta)^2 \,.$$

So we have the claim verified by letting $\epsilon \to 0$. □

Assume that u_δ and u_0 are the solutions to (25) and (26) respectively. Let us denote $e_\delta(x) = u_\delta(x) - u_0(x)$ and $T_\delta(x) = (\mathcal{L}_0 u_0 - \mathcal{L}_\delta u_0) + (f_\delta^L - f)$, then $\mathcal{L}_\delta e_\delta(x) = \mathcal{L}_\delta u_\delta(x) - \mathcal{L}_\delta u_0(x) = T_\delta(x)$. By Taylor expansion and the symmetry of the kernels, we can get the following truncation error estimate.

Lemma 3.8 (Truncation error)**.** *Suppose u_0 is the solution to local problem (26). Then*

$$T_\delta(x) = \begin{cases} O(\delta^2) & \text{for } x \in [\delta, 1)\,, \\ \left(\int_x^\delta \left(2s^2x - \frac{s^3}{6} - 3x^2 s\right)\rho_\delta(s)ds\right)u_0'''(0) + O(\delta^2) & \text{for } x \in (0, \delta)\,. \end{cases}$$

To get the formal order of convergence, we need the following important lemma.

Lemma 3.9. *Suppose that a nonnegative continuous function $\Phi(x)$ is defined on $\Omega\cup\Omega_D$, and*

$$-\mathcal{L}_\delta \Phi(x) \ge G(x) > 0 \,.$$

Then

$$\sup_{x\in\Omega} |e_\delta(x)| \le \sup_{x\in\Omega_D} \Phi(x) \cdot \sup_{x\in\Omega} \frac{|T_\delta(x)|}{G(x)}$$

Proof. Let $K_\delta = \sup_{x\in\Omega} \frac{|T_\delta(x)|}{G(x)}$. Then consider $K_\delta\Phi(x) + e_\delta(x)$, we have $\mathcal{L}_\delta(K_\delta\Phi + e_\delta) \le 0$. By applying the maximum principle Lemma 3.7 (noticing that it can be applied since $u_\delta \in C(\overline{\Omega})$ if $f_\delta^L \in C(\overline{\Omega})$ which implies $e_\delta \in C(\overline{\Omega})$), we have

$$\sup_{x\in\Omega} e_\delta(x) \le \sup_{x\in\Omega}(K_\delta\Phi(x) + e_\delta(x)) \le \sup_{x\in\Omega_D}(K_\delta\Phi(x) + e_\delta(x)) = K_\delta \sup_{x\in\Omega_D} \Phi(x)\,,$$

where $e_\delta(x) = 0$ for $x \in \Omega_D$ is used. Similarly, we can also get

$$\sup_{x\in\Omega} -e_\delta(x) \le K_\delta \sup_{x\in\Omega_D} \Phi(x)\,,$$

which completes the proof. □

Now to find $\Phi(x)$, the so-called barrier function (as in the PDE literature), we suppose that it is of the form

$$\Phi(x) = x^2 + 2x\,.$$

Then $\Phi(x)$ is nonnegative on Ω_D. Moreover, let

$$G(x) = -\mathcal{L}_\delta\Phi(x) = \begin{cases} 2 & \text{for } x \in (\delta, 1)\,, \\ 2\int_{-x}^\delta \rho_\delta(s)\big(s^2 + 2sx + 2s\big)ds & \text{for } x \in [0, \delta]\,. \end{cases}$$

Therefore, $G(x) > 0$ for $x \in \Omega$ since when $x \in [0, \delta]$,

$$G(x) = 2\int_{-x}^\delta \rho_\delta(s)s^2 ds + 4(1+x)\int_x^\delta \rho_\delta(s)s ds > 0\,.$$

Now if we pick a specific kernel, namely (6) with γ being the characteristic function on (0, 1):

$$\rho_\delta(x, x') = \frac{3}{2\delta^3}\chi_{[0,1]}\left(\frac{|x-x'|}{\delta}\right) \quad \text{for all } x, x' \in \mathbb{R}. \tag{27}$$

Then we have

$$K_\delta = \sup\left\{\sup_{x\in(0,\delta)} \frac{|\delta^4 - 16\delta^3 x - 36\delta^2 x^2 + 51x^4||u_0'''(0)| + O(\delta^4)}{16\big(\delta^3 + 3\delta^2(1+x) - x^2(3+2x)\big)}, O(\delta^2)\right\},$$

where the first term can be proved to be $O(\delta^2)$. Indeed, let $x = \alpha\delta$, $\alpha \in (0, 1)$, then the first term is equivalent to

$$\frac{(1-\alpha)|1-15\alpha-51\alpha^2-51\alpha^3||u_0'''(0)|\delta^4+O(\delta^5)}{48\big(1-\alpha^2\big)\delta^2+\mathcal{O}(\delta^3)} = O(\delta^2)\,.$$

Combining Lemma 3.9 and the above calculations, we have the desired $O(\delta^2)$ estimate.

More generally, for rescaled kernels (6), we have

$$K_\delta = \sup\left\{ \sup_{x\in(0,\delta)} \frac{\left|\int_x^\delta \rho_\delta(s)\big(2s^2x - \frac{s^3}{6} - 3x^2s\big)ds\right|}{\int_{-x}^\delta \rho_\delta(s)(2s+2sx+s^2)ds}|u_0'''(0)|, O(\delta^2)\right\}.$$

Let $x = \alpha\delta$ where $\alpha \in (0, 1)$. We can simplify the fraction in the above equation by plugging (6) into it and apply a change of variable $t = s/\delta$ to get:

$$\frac{\left|\int_x^\delta \rho_\delta(s)\big(2s^2x - \frac{s^3}{6} - 3x^2s\big)ds\right|}{\int_{-x}^\delta \rho_\delta(s)(2s+2sx+s^2)ds} = \delta^2\cdot\frac{\left|\int_\alpha^1 \gamma(s)\big(2\alpha s^2 - \frac{s^3}{6} - 3\delta\alpha^2s^2\big)ds\right|}{\int_{-\alpha}^1 \gamma(s)(2s+2\alpha\delta s+\delta s^2)ds}\,,$$

which can be proved to be $O(\delta^2)$. Indeed, by (14) we can get

$$\int_{-\alpha}^1 \delta s^2\gamma(s)ds = O(\delta)\,.$$

Moreover, the numerator on the right hand side

$$\begin{aligned}\left|\int_\alpha^1 \gamma(s)\left(2\alpha s^2 - \frac{s^3}{6} - 3\delta\alpha^2s^2\right)ds\right| &\le (2\alpha+3\delta\alpha^2)\int_\alpha^1 \gamma(s)s^2ds + \frac{1}{6}\int_\alpha^1 \gamma(s)s^3ds\\ &\le \left(2\alpha+3\delta\alpha^2+\frac{1}{6}\right)\int_\alpha^1 \gamma(s)sds\,.\end{aligned}$$

and the denominator can be simplified to

$$\int_{-\alpha}^1 \gamma(s)(2s+2\alpha\delta s+\delta s^2)ds = (2+2\alpha\delta)\int_\alpha^1 \gamma(s)sds + O(\delta)\,.$$

Then there exists a constant C independent of δ and α, such that

$$\frac{\left|\int_\alpha^1 \gamma(s)\left(2\alpha s^2 - \frac{s^3}{6} - 3\delta\alpha^2s^2\right)ds\right|}{\int_{-\alpha}^1 \gamma(s)(2s+2\alpha\delta s+\delta s^2)ds} \le C\,,$$

which again gives the $O(\delta^2)$ convergence order. We summarize in to the following key result of this paper.

Theorem 3.10. *Suppose u_δ solves the nonlocal problem (25) and u_0 is the solution to local problem (26). Then when $\delta < \delta_0$ for some constant δ_0, there exists a constant $C > 0$ independent of δ such that*

$$\sup_{x\in\Omega}|u_\delta(x) - u_0(x)| \le C\delta^2\,.$$

3.3. Inhomogeneous Neumann conditions

Now we discuss the nonlocal analog to the classical diffusion problem with inhomogeneous Neumann boundary conditions. The latter is given by

$$\begin{cases}\mathcal{L}_0u = f & \text{in }\Omega\,,\\ u'(0) = a\,, & u(1) = 0\,,\end{cases} \tag{28}$$

where $a \neq 0$.

We aim to impose Neumann type volume constraint at the left end point $x = 0$. In order to have the consistency, we assume in addition that the first moment of γ exists for any $\delta > 0$, namely

$$\int_0^1 \gamma(s)s\,ds < \infty\,. \tag{29}$$

Note that (29) may not hold for all kernels given by (6), for example, $\gamma(s) = 1/s^2$. However, among practical choices of γ, one often takes it to be integrable in many numerical simulations, then (29) is automatically satisfied.

Instead of (25), the nonlocal equation to be solved is

$$\begin{cases} \mathcal{L}_\delta u = \tilde{f}^L_\delta & \text{on } \Omega\,, \\ u = 0 & \text{on } \Omega_D\,, \end{cases} \tag{30}$$

where $\mathcal{L}_\delta$ remains the same as (24) but

$$\tilde{f}^L_\delta(x) = f^L_\delta(x) + 2a\int_{-\delta}^{0} \rho_\delta(x,x')(x'-x)dx'\,. \tag{31}$$

By (30), it is easy to check that the extra integration in (32) is well defined since $\gamma(s)$ does not have singularities when $x \neq 0$. Moreover, Lemma 3.8 and Lemma 3.9 still hold in this case since the last term in (32) cancels the new terms of truncation errors due to the inhomogeneous conditions. Therefore, we still have the following result.

Theorem 3.11. *Suppose u_δ solves the nonlocal problem (31) and u_0 is the solution to local problem (29). Then when $\delta < \delta_0$ for some constant δ_0, there exists a constant C independent of δ such that*

$$\sup_{x\in\Omega} |u_\delta(x) - u_0(x)| \le C\delta^2\,.$$

Remark 1. We can generalize the last term in (32). Indeed, to solve for inhomogeneous Neumann boundary conditions, we introduce an auxiliary function u_b which is supported on $(-\delta, 0)$. Define

$$\mathcal{L}^N_\delta u_b = -2\int_{-\delta}^{0} \rho_\delta(x,x')(u_b(y) - u_b(x))dy\,.$$

Then (32) can be written as

$$\tilde{f}^L_\delta(x) = f^L_\delta(x) + 2\mathcal{L}^N_\delta u_b\,,$$

where $u_b(x) = -ax$ for $x \in (-\delta, 0)$. Here $a \neq 0$ is the local Neumann boundary data and the negative sign comes from the outward normal direction at $x = 0$. The work [12] also discussed how to impose the inhomogeneous nonlocal Neumann conditions, which shares some similarities with the discussions here.

In general, u_b does not have to be a linear function and the kernel in $\mathcal{L}^N_\delta$ does not have to be the same as that in $\mathcal{L}_\delta$. It is sufficient to choose the kernel β_δ for $\mathcal{L}^N_\delta$ and the auxiliary function u_b such that

$$\int_{-\delta}^{0} \beta_\delta(x,x')(u_b(x') - u_b(x))dx' = a\int_{-\delta}^{0} \rho_\delta(x,x')(x'-x)dx' + \mathcal{O}(\delta)\,, \tag{32}$$

where $\mathcal{O}(\delta)$ is some higher order term that is at least uniformly bounded by a constant multiple of δ. We note that one can use a similar approach to solve inhomogeneous Neumann problems in high dimensional spaces, details will be presented in a separate work.

4. Numerical schemes

In this section, two classes of discrete schemes for (16) are studied, including the quadrature/collocation schemes which are analogous to the ones presented in [33], and conforming finite element Galerkin approximations with piecewise constant and piecewise linear finite element spaces. We refer to [7,11,34,36] for more discussions on different numerical schemes and additional references. In this and the followed section we still use the kernel (27) which provides a good illustration of the more general case without messy notations.

4.1. Geometric discretization

We consider a uniform mesh (grid) in this section. For a positive integer N, we set $h = 1/N$ and let $\delta = rh$ for an integer $r \ge 1$. Furthermore, we assume $\delta < \frac{1}{3}$. Introduce grid points on Ω as $\{x_i = (i-1)h\}_{i\in\Omega_N}$ where the index set is defined by $\Omega_N = \{1, 2, \dots, N+1\}$. Denote by $I_j = ((j-1)h, jh)$ for $1 \le j \le r$. We also define the standard piecewise constant basis functions by

$$\phi^0_i(x) = \begin{cases} 1 & \text{for } x \in (x_{i-1}, x_i), \\ 0 & \text{otherwise}, \end{cases} \qquad \text{for } i \in \Omega_N, \tag{33}$$

and the standard continuous piecewise linear *hat* basis functions by

$$\phi^1_i(x) = \begin{cases} (x - x_{i-1})/h & \text{for } x \in (x_{i-1}, x_i), \\ (x_{i+1} - x)/h & \text{for } x \in [x_i, x_{i+1}), \\ 0, & \text{otherwise} \end{cases} \qquad \text{for } i \in \Omega_N. \tag{34}$$

4.2. Quadrature based finite difference discretization

For $x \in \Omega_\delta$, since the integrating interval is symmetric with respect to x, we can follow [33] to get

$$\mathcal{L}_\delta u(x) = \int_0^\delta \rho(s)(u(x-s) - 2u(x) + u(x+s))ds$$
$$= \int_0^\delta \frac{u(x-s) - 2u(x) + u(x+s)}{s^\alpha} s^\alpha \rho_\delta(s)ds. \tag{35}$$

We consider the discrete operator $\mathcal{L}^h_{\delta,\alpha}$ given by

$$\mathcal{L}^h_{\delta,\alpha} u_i = \sum_{m=1}^{r} \frac{u_{i-m} - 2u_i + u_{i+m}}{(mh)^\alpha} \int_{I_m} s^\alpha \phi_i^1(s)\rho_\delta(s)ds. \quad i = r+1, \dots, N-r, \tag{36}$$

where $\{u_i\}$ are approximations of $\{u(x_i)\}$.

If we take α to be 1, then the discrete operator above can be written by

$$\mathcal{L}^h_{\delta,0} u_i = -\frac{3h}{\delta^3} \sum_{m=1}^{r-1} (u_{i-m} - 2u_i + u_{i+m}) - \frac{h^2(3r-1)}{2\delta^4}(u_{i-r} - 2u_i + u_{i+r}), \tag{37}$$

for $i = r+1, \dots, N-r$.

In [33], it was shown that such quadrature-based schemes are asymptotically compatible for linear nonlocal equations with Dirichlet-type constraints. We now demonstrate in our numerical experiments that it is also true for Neumann volume-constrained problems.

A distinction from [33] is that we also need to discuss here the case that $x \in \Omega \backslash \Omega_\delta$, for which the integrating interval is no longer symmetric. We can either directly use the composite trapezoid rule to approximate the integral, or separate the interval into a symmetric part where we can again exploit the quadrature scheme mentioned above and the remainder where we can consider other quadratures. The details are omitted.

Given the above discrete nonlocal difference operators, the proposed quadrature based finite difference scheme of (16) is

$$-\mathcal{L}^h_{\delta,0} u_i = f_\delta(x_i) \quad i \in \{1, \dots, N+1\} \tag{38}$$

Let $\mathbf{U}$ be a column vector with entries $\{u_i\}_{i=1}^{N+1}$, and $\mathbf{F}$ be that with entries $\{f_\delta(x_i)\}_{i=1}^{N+1}$, we may rewrite the corresponding linear systems as

$$\mathbb{A}_D \mathbf{U} = \mathbf{F}. \tag{39}$$

Note that the above stiffness matrix is obtained without any compatibility constraints, so the matrix is singular and the solution of corresponding linear system is not unique. This issue is to be discussed in Section 5.

4.3. Finite element discretization

Given the constrained energy space $\mathcal{S}_\delta(\Omega)$ and the bilinear form in Section 2.3, the associated weak formulation of (16) is given by: finding $u \in \mathcal{S}_\delta(\Omega)$ such that $\forall v \in \mathcal{S}_\delta(\Omega)$,

$$B(u, v) = (f_\delta, v)_\Omega.$$

Let $\mathcal{S}^h_\delta \subset \mathcal{S}_c$ be a family of finite element spaces corresponding to a uniform mesh $\{x_i\}$ parameterized by the mesh size h, as described earlier, with $\{\phi_i^k\}_{i=1}^{N_h}$ being the nodal basis. Let $u_h \in \mathcal{S}^h_\delta$ be the Galerkin approximation of u given by

$$B(u_h, v_h) = (f_\delta, v_h)_\Omega \quad \forall v_h \in \mathcal{S}^h_\delta\ . \tag{40}$$

Now suppose $u_h = \sum_{i=1}^{N_h} u_i\phi_i^k(x)$, we pay particular attention to the cases $k = 0$ and 1 with the case $k = 0$ corresponding to piecewise constant basis functions (34) (if the energy space admits such functions, which is guaranteed if ρ_δ has finite first order moment), and the case $k = 1$ corresponding to standard continuous piecewise linear elements with *hat* basis functions given by (35) (which works for ρ_δ that has finite second order moment).

Similar to difference approximations, let $\mathbf{U}$ be the column vector composed of the nodal values $\{u_i\}_{i=1}^{N_h}$, and $\mathbf{F}^k$ being the vector with entries $\{(f_\delta, \phi_i^k)_\Omega/h\}_{i=1}^{N_h}$ that represent the weighted average of f_δ around x_i. Then (41) gives linear systems $\mathbb{A}_{E,k}\mathbf{U} = \mathbf{F}^k$ with $\{\mathbb{A}_{E,k}\}_{k=0}^1$ being the nonlocal stiffness matrices for the finite element approximation. The issue of uniqueness of solution will again be discussed later.

5. Numerical studies

We now report results of numerical experiments which substantiate the analysis given earlier and offer quantitative pictures to the behavior of numerical solutions especially in the local limit. We first discuss how to impose the Neumann constraint numerically in order to ensure the uniqueness of the numerical solution. The order of convergence for some limiting processes are also examined. Through the numerical experiments, we can recover results analogous to those in [33] for pure Dirichlet constraints. The kernel used in this section is again taken as (27).

Table 1
Errors of quadrature collocation and piecewise finite element approximations for fixed $\delta = \frac{1}{4}$ to solution $x^4 - 2x^3 + x^2$.

	Quadrature collocation		p.w. linear fem	
h	$\|\mathbf{U}^h - \mathcal{R}_h u\|_\infty$	Order	$\|u^h - \mathcal{I}_h u\|_\infty$	Order
2^{-3}	4.59×10^{-3}	–	8.23×10^{-3}	–
2^{-4}	1.19×10^{-3}	1.95	3.85×10^{-3}	1.10
2^{-5}	3.00×10^{-4}	1.98	1.22×10^{-3}	1.66
2^{-6}	7.53×10^{-5}	1.99	3.37×10^{-4}	1.85
2^{-7}	1.88×10^{-5}	2.00	8.82×10^{-5}	1.93
2^{-8}	4.71×10^{-6}	2.00	2.25×10^{-5}	1.97
2^{-9}	1.18×10^{-6}	2.00	5.69×10^{-6}	1.98
2^{-10}	2.94×10^{-7}	2.00	1.43×10^{-6}	1.99

5.1. Numerically imposing the compatibility constraints

After numerical discretization, we get the stiffness matrices $\mathbb{A}$ that can be $\mathbb{A}_D$, $\mathbb{A}_{E,0}$ or $\mathbb{A}_{E,1}$. However, they all have a one-dimensional kernel due to the non-uniqueness. We may impose the constraint that the average of the solution being zero. Or we may modify the stiffness matrix obtained from numerical discretization. Let $\mathbb{E}$ be the column vector with entries all 1. Then $\mathbb{E}$ is in the kernel of stiffness matrix $\mathbb{A}$. Let $\mathbb{B} = \mathbb{A} + \mathbb{E}\mathbb{E}^T$, we solve the linear system $\mathbb{B}\mathbf{U}' = \mathbf{F}$ instead of solving $\mathbb{A}\mathbf{U} = \mathbf{F}$, where $\mathbf{F}$ is the right hand side corresponding to different stiffness matrices. Then the vector $\mathbf{U}'$ has the property of mean zero. For homogeneous nonlocal Neumman condition, $\mathbf{U}'$ is the numerical solution we want. If the compatibility constraint is that average of u in (0, 1) is C_n but not zero, we need to set $\mathbf{U}^h = \mathbf{U}' + C_h\mathbb{E}$, where $C_h \to C_n$ as $h \to 0$ (h is the mesh size).

In our experiments, we adopt the second approach for the following reasons: (1) the order of convergence with mixed type volume constraints is derived theoretically in Section 3.2. We want to see if there is any difference for pure Neumann volume constraints; (2) previous studies in [33] contained a set of experiments with Dirichlet volume constraints, it is desirable to impose pure Neumann type constraints numerically as in the model here in order to compare with the results shown in [33].

We note that the compatibility constraint can be avoided if we impose Dirichlet type volume constraint on one end of the nonlocal boundary region ($\Omega_D = [1, 1+\delta]$, for instance) and consider Neumman type constraint on the other end. In other words, we discretize and solve (25) with the nonlocal operator given by (24). This also ensures the uniqueness of the numerical solution without the need for imposing the compatibility constraint.

5.2. Example 1

We first fix the horizon δ. In order to get simpler benchmark solutions, we calculate the right hand side of the nonlocal equation based on an exact solution $u(x) = x^2(1-x)^2$. This naturally leads to a δ-dependent right hand side $f = \tilde{f}_\delta(x)$. Meanwhile, we need to modify our nonlocal constraints to match with $u(x)$, which leads to our target inhomogeneous volume constrained equation:

$$\begin{cases} \mathcal{L}_\delta u = \tilde{f}_\delta \quad \text{on } \Omega\,, \\ \int_\Omega u = C_n\,. \end{cases} \tag{41}$$

We solve the nonlocal problem on a uniform mesh and take δ to be constant and reduce h to check the convergence properties. As an illustration we choose $\delta = \frac{1}{4}$ and refine the mesh with decreasing h. For each h, we use the second approach discussed above to numerically impose the compatibility conditions and the constant C_h is chosen as $C_h = C_n = \frac{1}{30}$ which is the integral of u over Ω.

Table 1 shows errors and error orders of the finite difference (columns 2 and 3) and the piecewise linear finite element (columns 4 and 5) approximations to limiting solution $x^2(1-x)^2$ with a fixed $\delta = \frac{1}{4}$ while refining mesh with a decreasing h, where $\mathcal{R}_h$ denotes the restriction to the quadrature points $\{x_i = ih\}_{i=0}^N$ and $\mathcal{I}_h$ denotes the piecewise linear interpolant operator. From the data in the table, we see that the convergence rate for fixed δ is $\mathcal{O}(h^2)$ for both finite difference and finite element approximations. We remark that the piecewise constant finite element approximation has the same convergence behavior and the data is omitted.

5.3. Example 2

We now report numerical experiments to show the order of convergence at continuum level as $\delta \to 0$, which was discussed analytically in Section 3. We discretize and solve the following equation:

$$\begin{cases} \mathcal{L}_\delta u_\delta = f_\delta \quad \text{on } \Omega\,, \\ \int_\Omega u_\delta = C_\delta\,. \end{cases} \tag{42}$$

Table 2
Errors and error orders of finite difference and piecewise linear finite element approximations as $\delta \to 0$ to solution $x^3/3 - x^6/6$.

	Quadrature collocation		p.w linear fem	
δ	$\|\mathbf{U}_\delta^h - \mathcal{R}_h u\|_\infty$	Order	$\|u_\delta^h - \mathcal{I}_h u\|_\infty$	Order
2^{-2}	3.03×10^{-2}	–	2.80×10^{-2}	–
2^{-3}	7.26×10^{-3}	2.06	5.07×10^{-3}	2.47
2^{-4}	1.79×10^{-3}	2.02	9.50×10^{-4}	2.41
2^{-5}	4.45×10^{-4}	2.01	1.92×10^{-4}	2.31
2^{-6}	1.08×10^{-4}	2.04	4.13×10^{-5}	2.21
2^{-7}	2.59×10^{-5}	2.06	8.48×10^{-6}	2.27

Table 3
Errors and error orders of finite difference and piecewise linear finite element approximations as $h \to 0$ with fixed $r = 2$ to solution $x^3/3 - x^6/6$.

	Quadrature collocation		p.w linear fem	
h	$\|\mathbf{U}_\delta^h - \mathcal{R}_h u\|_\infty$	Order	$\|u_\delta^h - \mathcal{I}_h u\|_\infty$	Order
2^{-3}	4.97×10^{-3}	–	1.13×10^{-2}	–
2^{-4}	1.20×10^{-3}	2.04	2.86×10^{-3}	1.98
2^{-5}	2.96×10^{-4}	2.02	7.21×10^{-4}	1.99
2^{-6}	7.34×10^{-5}	2.01	1.81×10^{-4}	2.00
2^{-7}	1.83×10^{-5}	2.01	4.53×10^{-5}	2.00
2^{-8}	4.55×10^{-6}	2.00	1.13×10^{-5}	2.00

f_δ is the modified body force given in (15). The constant C_δ in the above equation is dependent of δ, and goes to some constant C_n when δ goes to zero, which means that the limiting local equation is

$$\begin{cases} \mathcal{L}_0 u = f \quad \text{on } \Omega\,, \\ u'(0) = u'(1) = 0\,, \\ \int_\Omega u = C_n\,. \end{cases} \tag{43}$$

We specify the local limit of the nonlocal solution as $u(x) = x^3/3 - x^6/6$, hence the right hand side of the local PDE would be $f(x) = 5x^4 - 2x$. Denote by $\mathbf{U}_\delta^h$ the numerical solution of (43) with horizon δ and mesh size h. Then from example 1, with fixed δ, $\mathbf{U}_\delta^h$ are known to converge to the interpolant of nonlocal solution u_δ with decreasing h. Therefore, when we keep δ decreasing and pick a relative small enough h as our limit case, the result we get can approximate the limiting process which we discussed in Section 3. In this example, since we only care about the limiting behavior of the numerical solution of u_δ, we can directly choose C_δ as $\frac{5}{84}$ which is the exact integral of the local limit u. Moreover, we impose such a constraint on the numerical solution $\mathbf{U}_\delta^h$ as well by setting

$$h(\mathbf{U}_\delta^h[1]/2 + \mathbf{U}_\delta^h[2] + \ldots + \mathbf{U}_\delta^h[N] + \mathbf{U}_\delta^h[N+1]/2) = 5/84.$$

Table 2 shows errors and error orders to the local limit of the quadrature collocation (columns 2 and 3) and piecewise linear finite element (columns 4 and 5) approximations as δ goes to 0 while fixing a small enough mech size h. From the data in the table, we can see that the convergence rate to the local limit is $O(\delta^2)$, which is same as what we showed in earlier analysis. We remark that the piecewise constant finite element approximations also converge to the local limit with the same rates.

We also want to check the asymptotic compatibility of the model. Table 3 shows that the error orders as $h \to 0$ with a fixed $r = \delta/h$ remain $\mathcal{O}(h^2)$.

Furthermore, we now confirm that the nonlocal solution recovers the Neumann boundary conditions as $\delta \to 0$ and the derivatives also converge. For $\mathbf{U}_\delta^h$ with different δ and h small enough, we have that

$$u'_\delta(0) \approx D_h^+ \mathbf{U}_\delta^h[1] := (\mathbf{U}_\delta^h[2] - \mathbf{U}_\delta^h[1])/h$$

and

$$u'_\delta(1) \approx D_h^- \mathbf{U}_\delta^h[N+1] := (\mathbf{U}_\delta^h[N+1] - \mathbf{U}_\delta^h[N])/h\,,$$

where $D_h^\pm$ are the difference quotient operators associated to forward and backward differences respectively. Central difference quotient is used for other nodes, namely

$$u'_\delta((j-1)h) \approx D_h \mathbf{U}_\delta^h[j-1] := (\mathbf{U}_\delta^h[j] - \mathbf{U}_\delta^h[j-2])/2h\,,$$

where $j = 2, 3, \ldots, N$. Take the finite difference approximation as illustration, Table 4 shows that as $\delta \to 0$, the derivatives of nonlocal solutions converge with an order of $\mathcal{O}(\delta)$. For more studies on nonlocal gradient recovery, we refer to [20].

Table 4
Errors and error orders of numerical derivatives of finite difference approximations as $\delta \to 0$.

δ	$\|D_h \mathbf{U}_\delta^h - \mathcal{R}_h u'\|_\infty$	Order
2^{-2}	4.51×10^{-1}	–
2^{-3}	2.24×10^{-1}	1.01
2^{-4}	1.17×10^{-1}	0.93
2^{-5}	6.09×10^{-2}	0.95
2^{-6}	3.11×10^{-2}	0.97
2^{-7}	1.57×10^{-2}	0.98

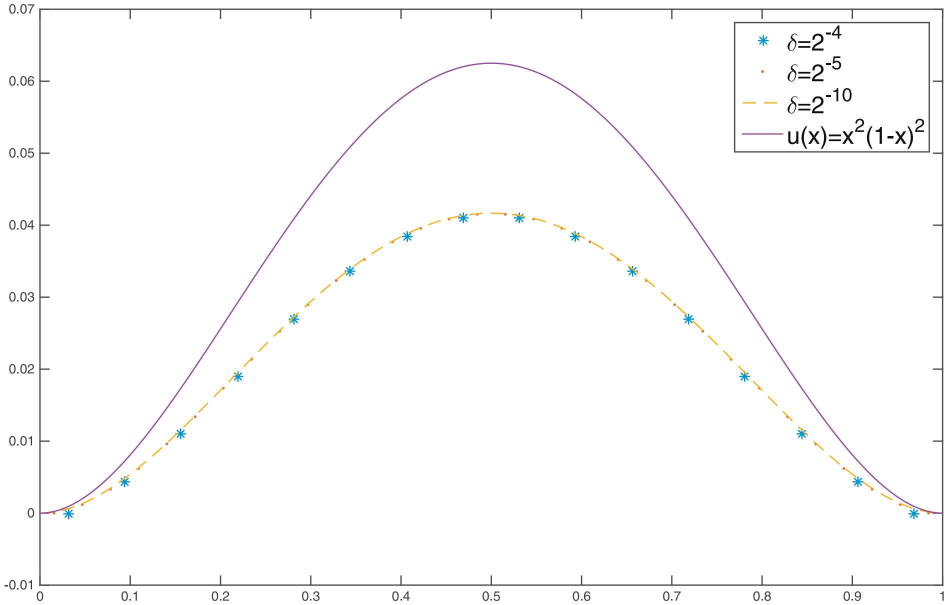

Fig. 1. The local limit of piecewise constant finite element approximation with fixed r as $h \to 0$.

5.4. Example 3

In this example, we study another limit process. Recall in [33,34] that in the case with asymptotically compatible finite difference and piecewise linear finite element discretization, the numerical solutions give the correct local limit but not the case with piecewise constant finite element. For $\delta = rh$ with a fixed integer $r \geq 1$, the continuous piecewise linear finite element approximation provides a consistent difference approximation to the local limit as $h \to 0$. Moreover, for problems with sufficiently smooth solutions, the order of truncation error is still $\mathcal{O}(h^2)$. However, for the piecewise constant finite element approximation, it goes to a different and wrong local limit as $h \to 0$, confirming that the conclusions in [33,34] remain valid for the Neumann case. We take $r = 1$ and start with $\delta = 2^{-4}$ and choose the local limit as $u(x) = x^2(1-x)^2$. Fig. 1 shows that with fixed $r = 1$, the piecewise constant finite element approximation converges to a local limit which is no longer u.

5.5. Discussions

The numerical experiments reported here are mostly restricted to smooth solutions. We leave experiments involving singular solutions and more general limits to future works. Based on the results of this section, we see that it is possible to recover most of the results in [33,34] where nonlocal diffusion and linear peridynamic models with Dirichlet type volume constraints and a constant horizon have been studied. We also note that similar studies for spatially changing horizon can also be done, which will be shown in the future works.

6. Conclusion and remarks

In this paper, we have analyzed a linear nonlocal diffusion model which is posed as a nonlocal boundary value problem of Neumann type. We have considered a class of kernels associated with the some variational problems. Basic structural properties of the associated nonlocal energy spaces, such as completeness and compactness, are established, leading to well-posedness for the variational problems. We refer to [21–23,25] for more properties of the energy space.

One of our main contributions in this work is a study of the limiting processes of both the nonlocal diffusion models and the discrete approximations, including the quadrature based finite difference and conforming finite element disircretizations. These are representatives of two classes of methods which can be applied to problems with very general nonlocal interaction kernels having a finite second order moment. Note that much of the previous studies on Dirichlet type constrained nonlocal diffusion problems have now been extended to problems with Neumann type volume constraints. We establish the local limit of the nonlocal diffusion model as the horizon goes to zero, and estimate the convergence rate of such a limiting process, which is confirmed by numerical experiments. In particular, we are able to numerically recover most of the results presented in [33] of the problems with Dirichlet volume constraints. In Section 5, we discuss the similarities and differences between the limiting behavior of numerical methods. These methods are all convergent with the same rate when applied to the nonlocal problem with a fixed horizon δ. However, they behave differently depending on the ratio of horizon and mesh size (δ/h) being fixed. The piecewise constant finite element approximation converges to a different local limit, which is a scalar multiple of the local limit of other approximations. The surprising findings are again consistent to the results given for models with homogeneous Dirichlet conditions.

Finally, the current study is largely based on a simple one-dimensional linear model for the sake of offering insight without being impeded by tedious calculations. In our analysis here, the computational mesh is taken to be uniform and the horizon parameter δ is also assumed to be a constant. While these serve the purpose of illustration well, additional complications may arise in practical implementations. In future works we plan to extend the results obtained in here to the linear peridynamic model with a spatially varying horizon which mimics a spatial change of scales in nonlocal interactions. The present work also serves as a useful step towards the study of nonlocal interface problems and the development of domain decomposition strategies for nonlocal problems.

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