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On Neumann-type Boundary Conditions for Nonlocal Models

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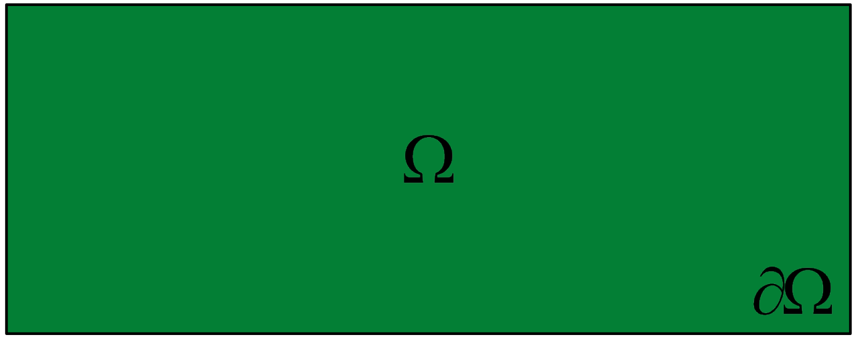
Local and Nonlocal Models and Boundaries

- Local model (i.e., PDEs)

$$-\nabla^2 u(x) = f(x) \quad x \in \Omega$$

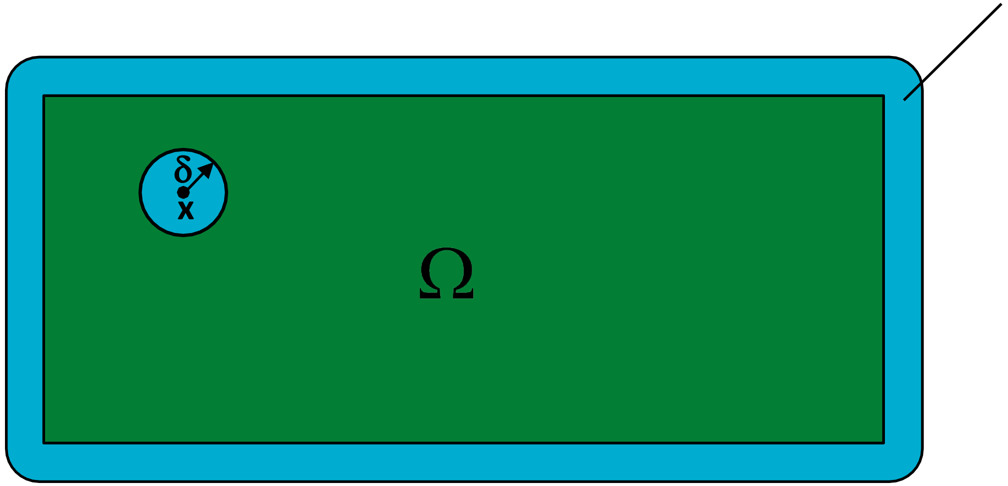
- Apply boundary conditions on boundary of domain (hence the name)



- Nonlocal model (i.e., integral equations)

$$\int_{B(x)} \big(u(y) - u(x)\big)\mu(y,x)dy \quad \text{for } x \in \Omega$$

- Nonlocal "boundary" is volumetric region, sometimes called "nonlocal boundary", "collar", etc.
- Boundary conditions for these models are called "nonlocal boundary conditions", "volume constraints", etc.



Nonlocal Calculus

- We will utilize the following operators from nonlocal calculus*,**

$$\alpha(x,y) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$$

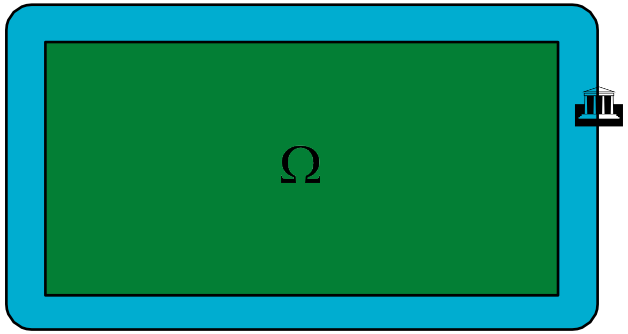
$$\mu(x,y) = \alpha(x,y) \cdot \alpha(x,y)$$

- Nonlocal point divergence

$$\mathcal{D}[\nu](x) = \int_{\Omega \cup \Gamma} \big(\nu(x,y)\cdot\alpha(x,y) - \nu(y,x)\cdot\alpha(y,x)\big)dy \quad \text{for } x \in \Omega$$

- Nonlocal two-point gradient

$$\mathcal{G}[u](x,y) = \big(u(y) - u(x)\big)\alpha(y,x) \quad \text{for } (x,y) \in \mathbb{R}^n \times \mathbb{R}^n$$



- Nonlocal normal operator

$$\mathcal{N}[\nu](x) = -\int_{\Omega \cup \Gamma} \big(\nu(x,y)\cdot\alpha(x,y) - \nu(y,x)\cdot\alpha(y,x)\big)dy \quad \text{for } x \in \Gamma$$

- Nonlocal Laplacian

$$\mathcal{L}[u](x) = \mathcal{D}\big[\mathcal{G}[u]\big](x) = 2\int_{\Omega \cup \Gamma} \big(u(y) - u(x)\big)\mu(y,x)dy \quad \text{for } x \in \Omega$$

*Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws, Mathematical Models and and Methods in Applied Sciences, 23 (2013), pp. 493-540.
** B. Hinds and P. Radu., Dirichlet's principle and wellposedness of steady state solutions for a nonlocal peridynamics model, Appl. Math. and Comput., 219 (2012), pp. 1411-1419.

Classical Neumann Boundary Value Problem

- Poisson equation with Neumann boundary conditions is energy minimizer of functional

$$E[u] = \int_{\Omega} \frac{1}{2} |\nabla u|^2 dx - \int_{\Omega} f(x)u(x)dx + \int_{\partial\Omega} g(x)u(x)d\sigma$$

$$\Downarrow$$

$$\begin{aligned} -\nabla^2 u(x) &= f(x) \qquad x \in \Omega \\ \nabla u \cdot n &= g(x) \qquad x \in \partial\Omega \end{aligned}$$

- Compatibility condition (necessary condition for solution existence):

$$\int_{\partial\Omega} g(x)\, dx = \int_{\Omega} f(x)\, dx$$

- Pure Neumann BVP is singular (constant function in kernel)
- Can solve numerically using (for example) Moore-Penrose Pseudoinverse, which gives minimum-norm solution.

Nonlocal Neumann Boundary Value Problem

- Many others* have observed analogous nonlocal energy

$$E[u] = \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} |\mathcal{G}u|^2\, dV_x\, dV_y - \int_{\Omega} u(x)\, f(x)\, dV_x + \int_{\Gamma} u(x)\, g(x)\, dV_x$$

- Using differentiation in Hilbert spaces and (nonlocal) integration by parts, compute

$$0 = \frac{d}{dt} E[u + tv]\Big|_{t=0}$$

$$= -\int_{\Omega}\left[\mathcal{L}[u](x) - f(x)\right]v(x)\, dV_x - \int_{\Gamma}\left[\int_{\Omega\cup\Gamma} 2\big(u(y)-u(x)\big)\mu(y-x)\, dV_y - g(x)\right]v(x)\, dV_x$$

- Which yields the nonlocal boundary value problem

$$-\mathcal{L}[u](x) = -\int_{\Omega\cup\Gamma}\left[u(y)-u(x)\right]\mu(y-x)\, dV_y = f(x), \quad x \in \Omega$$

$$\mathcal{N}[\mathcal{G}u](x) = 2\int_{\Omega\cup\Gamma}\left[u(y)-u(x)\right]\mu(y-x)\, dV_y = g(x), \quad x \in \Gamma$$

- **We desire this system to converge to its local counterpart for consistency with classical physics.**

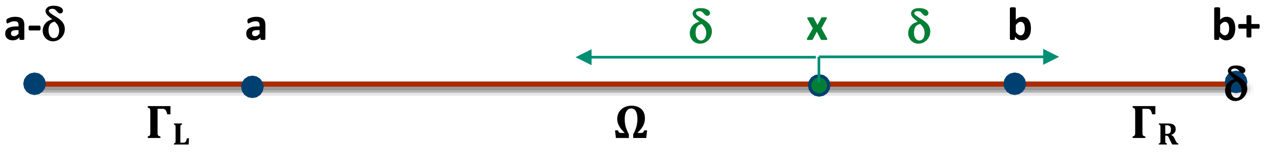
* Q. Du, M. Gunzburger, R. B. Lehoucq, and K. Zhou, Analysis and approximation of nonlocal diffusion problems with volume constraints, SIAM review, 54, 667-696, 2012.

Convergence of Nonlocal Laplacian

- Given an appropriate kernel μ, convergence has been oft-demonstrated

$$\lim_{\delta \to 0} \mathcal{L}[\mathbf{u}](\mathbf{x}) = \nabla^2 \mathbf{u}(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega$$

- Define 1D model



- Assume $\mu = 3 / \delta^3$; Compute Taylor series:

$$\frac{3}{\delta^3} \int_{x-\delta}^{x+\delta} [u(y) - u(x)]dy = u''(x) + \frac{\delta^2}{20} u^{(4)}(x) + \dots \qquad \text{for } x \in \Omega$$

- Domain of integration for all points $x \in \Omega$ is symmetric. Odd derivatives cancel.

- Moreover,

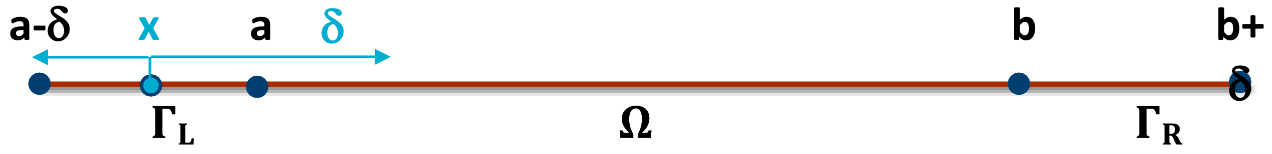
$$\left\| \mathcal{L}[\mathbf{u}](\mathbf{x}) - \nabla^2 \mathbf{u}(\mathbf{x}) \right\| = o(\delta^2)$$

Convergence of Nonlocal Neumann Operator

- ❑ Given same kernel μ, consider the convergence

$$\mathcal{N}[\mathcal{G}u](x) \rightarrow \frac{\partial u}{\partial n}(a) = u'(a) \qquad \text{for } x \in \Gamma_L,\; x \rightarrow a, \delta \rightarrow 0$$

- ❑ Define 1D model



- ❑ Assume $\mu = 3 / \delta^3$; Compute Taylor series.
- ❑ Domain of integration for all points $x \in \Gamma$ ***not*** symmetric. Odd derivatives do not cancel.

$$\frac{3}{\delta^3}\int_{a-\delta}^{x+\delta}\left[u(y) - u(x)\right]dy = \frac{3}{\delta^3}(a - x)(a - x - 2\delta)u'(x) + \mathrm{K} \qquad \text{for } x \in \Gamma_L$$

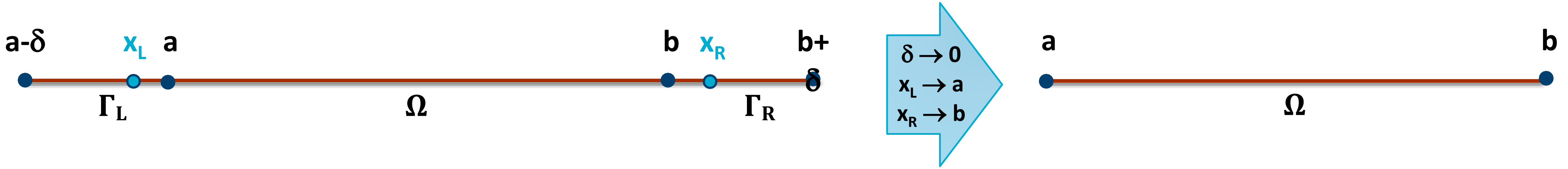
$$\approx \frac{1}{\delta}u'(x) + \mathrm{K}$$

Coefficient is x-dependent and divergent!

- ❑ Why the singularity?
  - ❑ The kernel μ was chosen to ensure nonlocal Laplacian converged to local Laplacian as $\delta \rightarrow 0$.
  - ❑ In general, nonlocal boundary (collar) must be treated differently than bulk for nonlocal models.
  - ❑ Variational approach scales nonlocal Neumann operator (collar) same as nonlocal Laplacian!

A New Type of Convergence

- Convergence of Neumann-type nonlocal operator to its differential equivalent as $\delta \to 0$ requires consideration of
  - Nonlocal Neumann operator evaluated at u(x), $x \in \Gamma$, where x varies as $|\Gamma| \to 0$
  - Rate at which any individual point $x \in \Gamma$ approaches $\partial\Omega$ as $\delta \to 0$
  - Operator-point condensated convergence; u(x) is fixed



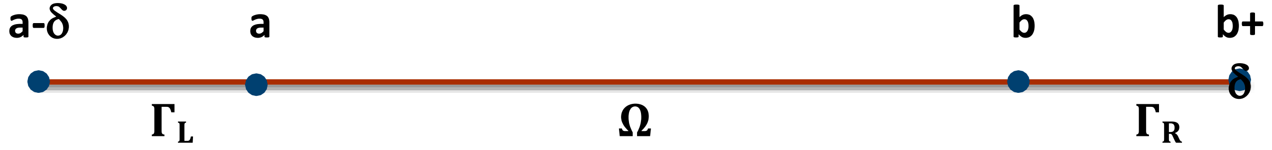
- Achieving desired convergence requires x-dependent scaling $\sigma(x,\mu)$.

$$\sigma_L(x,\mu)\mathcal{N}[\mathcal{G}u](x) \;\to\; \frac{\partial u}{\partial n}(a) = u'(a) \qquad \text{for } \; x \in \Gamma_L,\; x \to a,\, \delta \to 0$$

$$\sigma_R(x,\mu)\mathcal{N}[\mathcal{G}u](x) \;\to\; \frac{\partial u}{\partial n}(b) = u'(b) \qquad \text{for } \; x \in \Gamma_R,\; x \to b,\, \delta \to 0$$

Nonlocal Neumann Operator Convergence

- Consider convergence at the left endpoint of a 1D domain ($\delta \to 0$, $x \in (a-\delta, a)$, $x \to a$):



- Taylor series with remainder tells us

$$\sigma(x,\mu)\mathcal{N}[\mathcal{G}u](x) = \sigma(x,\mu)u'(x)\int_{a-\delta}^{x+\delta}(y-x)\mu(y-x)dy + \sigma(x,\mu)\int_{a-\delta}^{x+\delta}u''(\xi)\frac{|y-x|^2}{2}\mu(y-x)dy$$

- from which we conclude

$$\sigma(x,\mu) = \left(\int_{a-\delta}^{x+\delta}(y-x)\mu(y-x)dy\right)^{-1}$$

- If $x \to a$ proportionally to δ, then

$$\sigma(x,\mu)\mathcal{N}[\mathcal{G}u](x) = u'(x) + O(\delta)$$

- Asymmetry of integrand results in (at most) 1st order convergence in δ.
  - What does this mean for convergence of solutions?

Solution Convergence & Nonlocal Compatibility Condition

- **Correctly scaled and convergent nonlocal Neumann problem:**

$$-\mathcal{L}[u](x) = -\int_{\Omega\cup\Gamma} \left[u(y)-u(x)\right]\mu(y-x)\,dV_y = f(x), \qquad x\in\Omega$$

$$\mathcal{N}[\mathcal{G}u](x) = \int_{\Omega\cup\Gamma} \left[u(y)-u(x)\right]\mu(y-x)\,dV_y = \frac{g(x)}{\sigma(x,\mu)}, \qquad x\in\Gamma$$

- **Theorem: Let $u_\delta(x)$ and $u(x)$ be sufficiently smooth solutions to the nonlocal and local Neumann BVPs, respectively. Then there exists C >0 such that**

$$\left\|u_\delta(x)-u(x)\right\|_{L_2(\Omega)} \le C\delta^2$$

- **Remark #1: Solution convergence still second order even though operator convergence is first order!**

- **Remark #2: Neumann operator scaling unnecessary for homogeneous BVP (i.e., g(x) = 0).**

Nonlocal Neumann Boundary Value Problem Revisited

- **What went wrong before?**

$$E[u] = \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} |\mathcal{G}u|^2 \, dV_x \, dV_y - \int_{\Omega} u(x)\, f(x)\, dV_x + \int_{\Gamma} u(x)\, g(x)\, dV_x$$

Goes to zero as $\delta \to 0$!

- **Previous nonlocal energy functional scaled incorrectly …**
  - **… but scaling error only manifests for inhomogeneous BVPs!**

- **Correctly scaled nonlocal energy functional:**

$$E[u] = \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} |\mathcal{G}u|^2 \, dV_x \, dV_y - \int_{\Omega} u(x)\, f(x)\, dV_x + \int_{\Gamma} u(x)\, \frac{g(x)}{\sigma(x,\mu)}\, dV_x$$

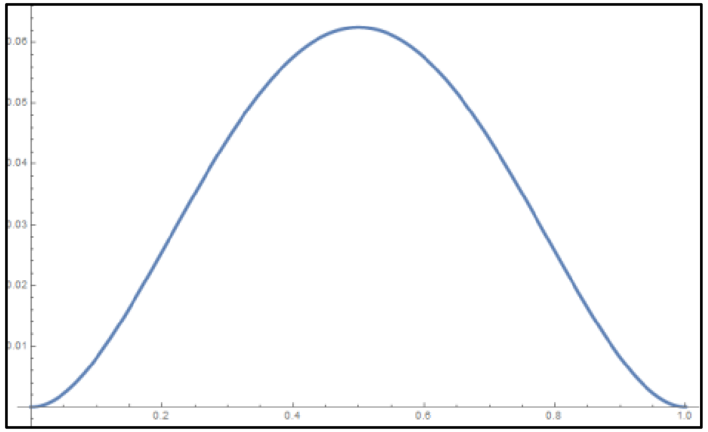
- **yields correctly scaled nonlocal boundary value problem**

$$-\mathcal{L}[u](x) = -\int_{\Omega\cup\Gamma} \left[u(y) - u(x)\right]\mu(y-x)\, dV_y = f(x), \qquad x \in \Omega$$

$$\mathcal{N}[\mathcal{G}u](x) = 2\int_{\Omega\cup\Gamma} \left[u(y) - u(x)\right]\mu(y-x)\, dV_y = \frac{g(x)}{\sigma(x,\mu)}, \qquad x \in \Gamma$$

Nonlocal Neumann BVP: Analytical Example

- What do solutions associated with nonlocal Neumann boundary conditions look like?
  - Given u(x) for $x \in \Omega$, if $\mu(y-x)$ constant we can solve analytically for u(x) for $x \in \Gamma$ (Fredholm Integral Equation of Second Kind)
  - This is not required for numerical solution; We do so here for curiosity
- Let
  - $u(x) = x^2 (1-x)^2, \; x \in \Omega = (0,1)$
  - $\delta = 0.1$
  - $\mathcal{N}[\mathcal{G}u](x) = 0, \; x \in \Gamma$
- Observations:
  - u(x), $x \in \Gamma$, is smooth except for discontinuity at boundary

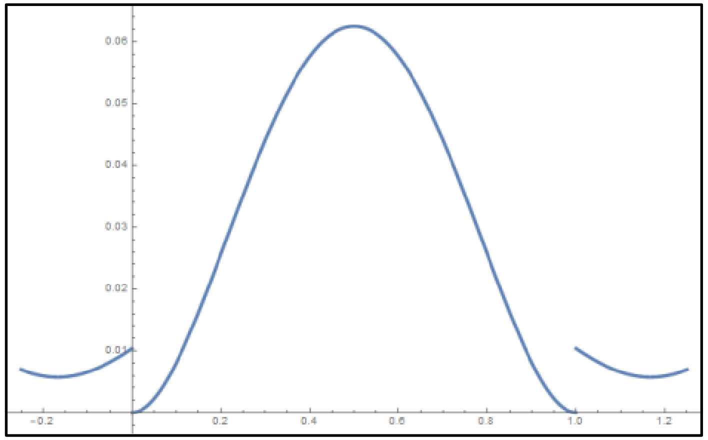


$$-\nabla^2 u(x) = f(x), \quad x \in \Omega$$
$$\nabla u(x) \cdot n = 0, \quad x \in \Gamma$$

Local Poisson's Equation

$$-\mathcal{L}[u](x) = f(x), \quad x \in \Omega$$
$$\mathcal{N}[\mathcal{G}u](x) = 0, \quad x \in \Gamma$$

Nonlocal Poisson's Equation



Nonlocal Neumann BVP: Computation

- Nonlocal Poisson's equation:

$$-\int_{x-\delta}^{x+\delta} \big(u(y)-u(x)\big)\,\mu(y-x)\,dy = f(x) \qquad x \in \Omega = (0,1)$$

$$\int_{-\delta}^{x+\delta} \big(u(y)-u(x)\big)\,\mu(y-x)\,dy = \frac{g_L(x)}{\sigma_L(x,\mu)} \qquad x \in \Gamma_L = (-\delta,0)$$

$$\int_{x-\delta}^{1+\delta} \big(u(y)-u(x)\big)\,\mu(y-x)\,dy = \frac{g_R(x)}{\sigma_R(x,\mu)} \qquad x \in \Gamma_R = (1,1+\delta)$$

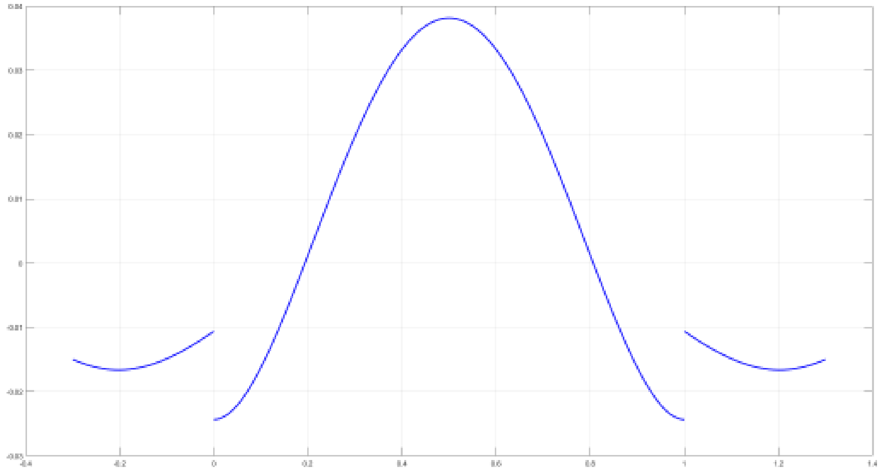
- Consider manufactured solution u(x)
  - Verify h-convergence
  - Verify δ-convergence

- Issue #1: Asymptotic incompatibility for certain discretizations*
  - Use piecewise linear discretization
- Issue #2: Solution may be discontinuous in $\Omega = (0,1)$, and definitely has discontinuity at x = 0,1.
  - Use discontinuous Galerkin discretization

* X. Tian and Q. Du, Asymptotically compatible schemes and applications to robust discretization of nonlocal models. *SIAM J. Numer. Anal.* 52, 1641–1665, 2014.

Example #1: Homogeneous Pure Neumann BVP

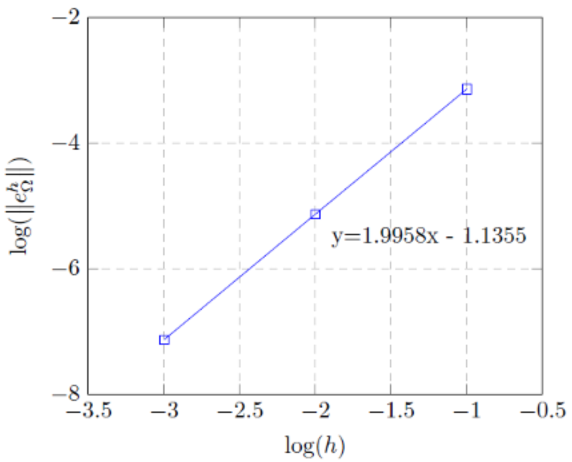
- Assume $\mu = 3 / \delta^3$, $g_L(x) = g_R(x) = 0$. Choice of $\sigma_L(x, \mu)$, $\sigma_R(x, \mu)$ does not matter!
- Let $u(x) = x^2(1-x)^2 - 1/30$, $x \in \Omega$
- Note that $u'(0) = u'(1) = 0$.



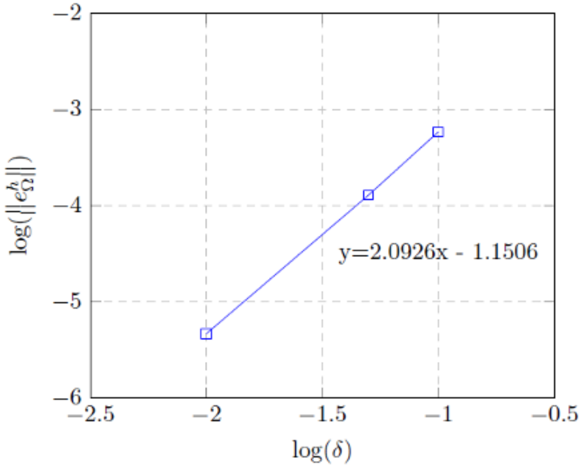
$$-\mu \int_{x-\delta}^{x+\delta} \big(u(y) - u(x)\big)\,dy = f(x) \qquad x \in \Omega = (0,1)$$

$$\mu \int_{-\delta}^{x+\delta} \big(u(y) - u(x)\big)\,dy = 0 \qquad x \in \Gamma_L = (-\delta, 0)$$

$$\mu \int_{x-\delta}^{1+\delta} \big(u(y) - u(x)\big)\,dy = 0 \qquad x \in \Gamma_R = (1, 1+\delta)$$



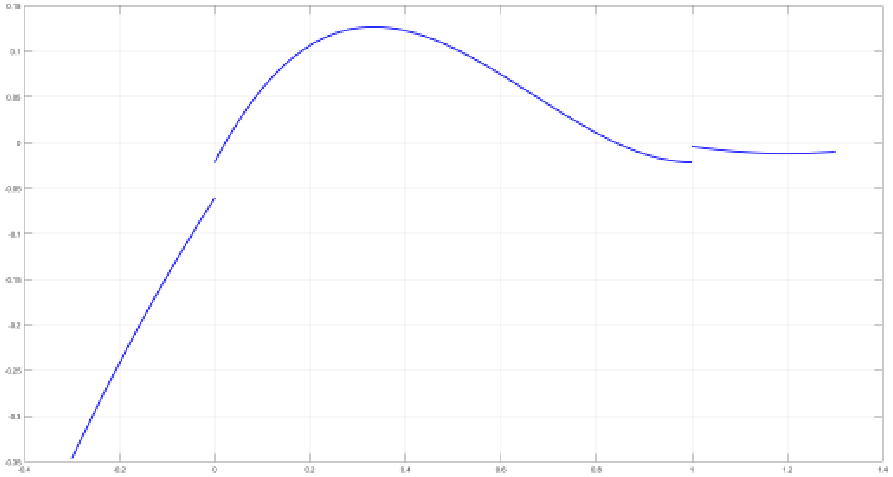
Log(error) vs. log(h), δ = 0.3



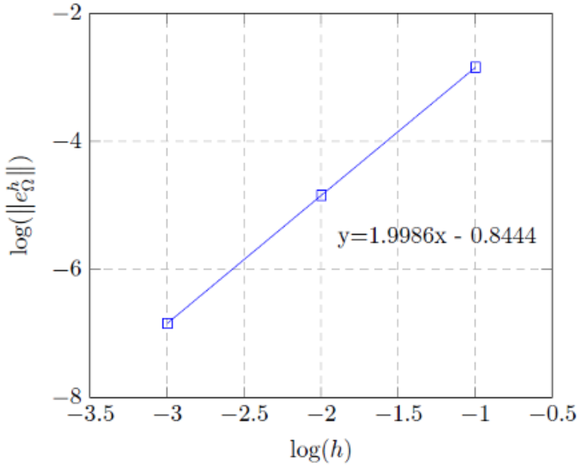
Log(error) vs. log(δ), h = 0.001

Example #2: Inhomogeneous Pure Neumann BVP

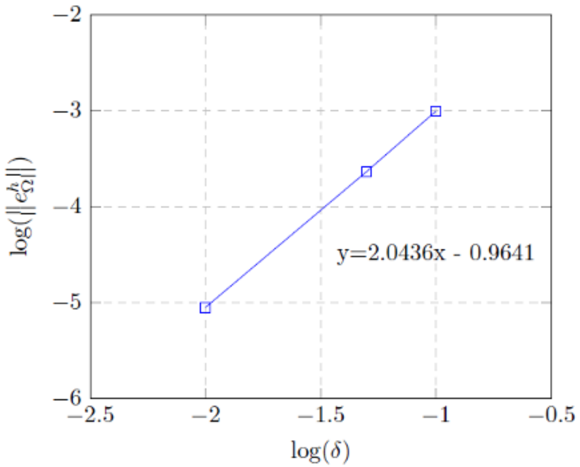
- Assume $\mu = 3 / \delta^3$, $g_L(x, \mu) = 1$; $g_R(x) = 0$. Implies $\sigma_L(x, \mu) = -2\delta^3/ (3x^2 + 6x\delta)$.
- Let $u(x) = x(1-x)^2 - 1/12$, $x \in \Omega$
- Note that $u'(0) = 1$; $u'(1) = 0$.



$$
\begin{aligned}
-\mu \int_{x-\delta}^{x+\delta} \big(u(y) - u(x)\big)\, dy &= f(x) & x &\in \Omega = (0,1) \\
\mu \int_{-\delta}^{x+\delta} \big(u(y) - u(x)\big)\, dy &= \frac{-(3x^2 + 6x\delta)}{2\delta^3} & x &\in \Gamma_L = (-\delta, 0) \\
\mu \int_{x-\delta}^{1+\delta} \big(u(y) - u(x)\big)\, dy &= 0 & x &\in \Gamma_R = (1, 1+\delta)
\end{aligned}
$$



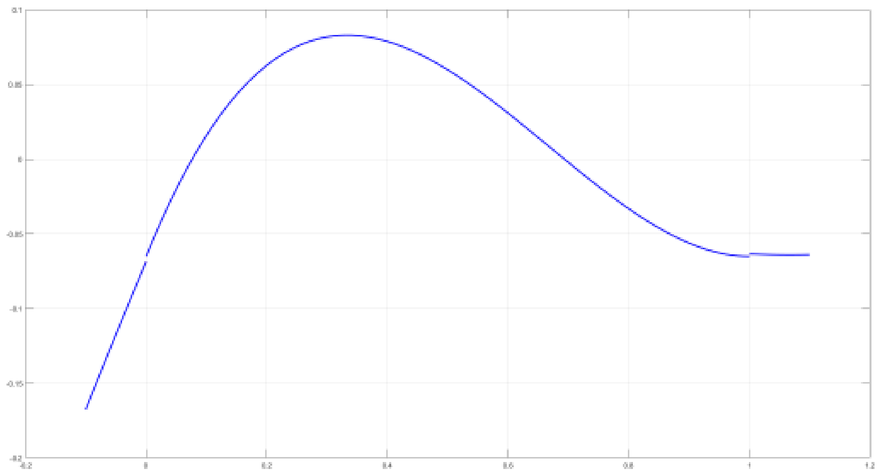
Log(error) vs. log(h), $\delta = 0.3$



Log(error) vs. log(δ), h = 0.001

Example #3: Inhomogeneous Pure Neumann BVP

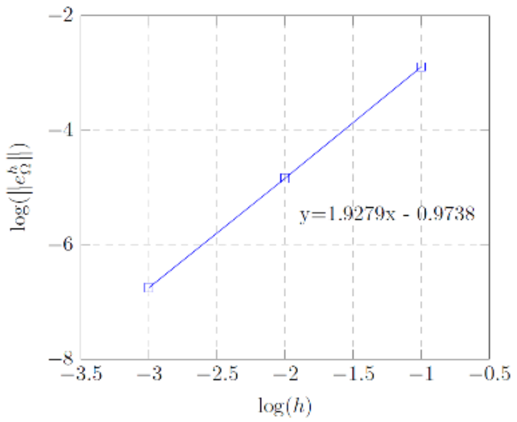
- **Assume $\mu(y-x) = -(s-3) / \delta^{3-s}|x-y|^s$; $g_L(x, \mu) = 0$; $g_R(x) = 0$. Choice of $\sigma_L(x, \mu)$, $\sigma_R(x, \mu)$ does not matter!**
- **Let $s=1/2$; Let $u(x) = x(1-x)^2 - 1/12$, $x \in \Omega$**
- **Note that $u'(0) = 1$; $u'(1) = 0$.**



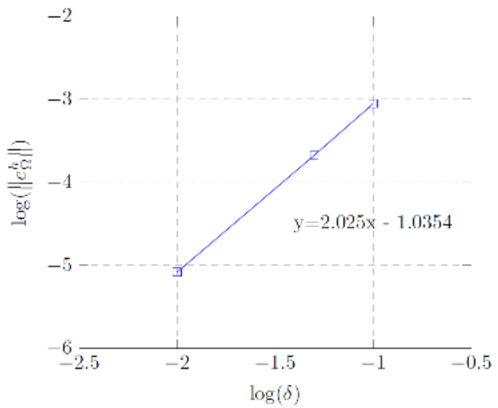
$$-\int_{x-\delta}^{x+\delta} \big(u(y)-u(x)\big)\,\mu(y-x)\,dy = f(x) \qquad x \in \Omega = (0,1)$$

$$\int_{-\delta}^{x+\delta} \big(u(y)-u(x)\big)\,\mu(y-x)\,dy = \frac{1}{\sigma_L(x,\mu)} \qquad x \in \Gamma_L = (-\delta,0)$$

$$\int_{x-\delta}^{1+\delta} \big(u(y)-u(x)\big)\,\mu(y-x)\,dy = 0 \qquad x \in \Gamma_R = (1,1+\delta)$$



Log(error) vs. log(h), δ = 0.3



Log(error) vs. log(δ), h = 0.001

Conclusions

- Demonstrated nonlocal Neumann operator consistent with local differential counterpart
  - Convergence must be considered differently than nonlocal Laplace operator
  - Results in position-dependent scaling

- Advantages
  - Consistent with local Neumann boundary condition
  - Implement and apply as easily as local boundary condition

- Questions?