A decoupled meshless Nyström scheme for 2D Fredholm integral equations of the second kind with smooth kernels

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(joint work with A. Sestini[1])

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Introduction

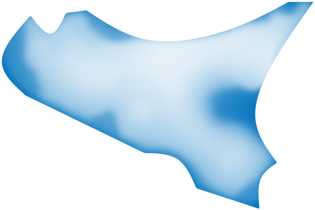
Introduction

Research topic

Numerical solution of integral equations. More specifically, Fredholm integral equations of the second kind in 2D with smooth kernels.

Real-world applications

Computation of equilibrium states for nonlocal diffusion equations. Such models arise in optics, material science, mathematical biology.



Example: equilibrium distribution of population subject to nonlocal dynamics on an island.

Introduction

Novelty of our work

We generalize classical Nyström schemes for the discretization of integral equations by decoupling solution nodes from quadrature nodes, in the same way that solution spaces and quadrature formulas are *naturally decoupled* in collocation or Galerkin schemes.

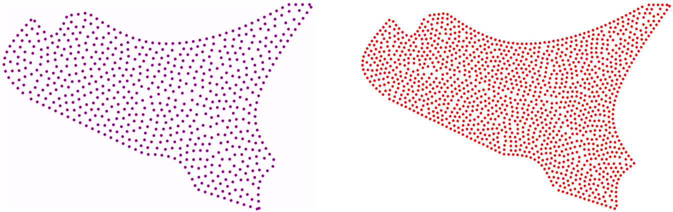


Figure: Coarse solution nodes (left) and fine quadrature nodes (right).

Introduction

Motivation for decoupling

In general, the decoupled Nyström method is more efficient than classical Nyström because it makes better use of degrees of freedom.

Fundamental intuition

Set of solution nodes: Determines the size of the linear system to be solved. It only has to be large enough to fully resolve the features of the smooth exact solution.

Set of quadrature nodes: Determines the size of the quadrature formula. It must be large enough to fully resolve the integral operator, whose integrands typically vary more rapidly than the exact solution.

Introduction

Prior work leading to decoupled Nyström

In [1], a novel way to determine stable, high-order quadrature weights for a given set of (reasonable) scattered nodes was introduced. Building on prior work, we adopted the meshless point of view when investigating Nyström methods. However, decoupling is not specific to meshless.

Motivation for meshless setting

When a high-order mesh is not available, choosing a good solution space for collocation and Galerkin methods can be hard. The Nyström method does not need a solution space, just solution nodes. Meshless lets us investigate decoupling under minimal assumptions on the nodes.

[1] Oleg Davydov and Bruno Degli Esposti (2025). *Meshless moment-free quadrature formulas arising from numerical differentiation*, CMAME.

Starting point: the classical Nyström method

Fredholm integral equations of the second kind

Let $\Omega \subset \mathbb{R}^d$ be a multivariate bounded domain.

We seek $u \in C^q(\overline{\Omega})$ such that

$$\lambda u(x) - \int_\Omega k(x,y)u(y)\,dy = f(x), \quad x \in \overline{\Omega},$$

for given $\lambda \neq 0$, rhs $f \in C^q(\overline{\Omega})$, and smooth kernel $k \in C^q(\overline{\Omega} \times \overline{\Omega})$.

In functional notation, the same equation is written as

$$(\lambda I - \mathcal{K})u = f$$

By the Fredholm alternative, it has a unique solution iff $\lambda \notin \sigma(\mathcal{K})$.

Numerical methods for integral equations

The main numerical methods for the solution of integral equations of the second kind are the collocation method, Galerkin method, degenerate kernel method, and Nyström method. In this talk we focus on the Nyström method, and try to overcome some of its limitations.

Consider a quadrature (aka cubature) formula

$$\sum_{i=1}^{|Y|} w_i v(y_i) \approx \int_\Omega v(y)\,dy, \quad v \in C^q(\overline{\Omega})$$

with nodes $Y \subset \overline{\Omega}$ and weights $w \in \mathbb{R}^{|Y|}$.

The Nyström method

Discretizing the integral term in Fredholm's equation leads to

$$\lambda u(x) - \sum_{i=1}^{|Y|} w_i k(x, y_i) u(y_i) = f(x), \tag{1}$$

a semidiscrete functional equation. Introducing the vector of unknowns $\hat{u} \approx u_{|Y}$ and imposing exactness of (1) for all $x \in Y$ gives the closed system of linear equations

$$\lambda \hat{u}_i - \sum_{j=1}^{|Y|} w_j k(y_i, y_j) \hat{u}_j = f(y_i), \quad i = 1, \dots, |Y|$$

This is the classical Nyström method.

The Nyström method

The linear system can be written more compactly as

$$A\hat{u} := (\lambda I - KW)\hat{u} = f_{|Y}$$

by introducing the matrices $(K)_{ij} = k(y_i, y_j)$ and $W = \operatorname{diag}(w)$.

The solution u can be approximated at any point $x \in \overline{\Omega}$ by Nyström's interpolation formula:

$$u(x) \approx \frac{1}{\lambda}\left(\sum_{i=1}^{|Y|} w_i k(x, y_i)\hat{u}_i + f(x)\right).$$

The accuracy of this approximation is proportional to the accuracy of the chosen quadrature formula.

The Nyström method

Advantages over collocation and Galerkin

Simpler implementation due to direct use of quadrature. Does not require the definition of a solution space.

Disadvantages over collocation or Galerkin

The size of the system matrix A (number of solution DOFs) is tied to the number of quadrature nodes $|Y|$. When the kernel is hard to integrate, Y cannot be refined locally.

Fundamental research questions in this work

Can we lift this limitation by decoupling solution nodes from quadrature nodes in Nyström's method? What advantages would this bring?

Decoupled Nyström method and error analysis

Decoupled Nyström method

Let us go back to the semidiscrete functional equation

$$\lambda u(x) - \sum_{i=1}^{|Y|} w_i k(x, y_i) u(y_i) = f(x).$$

Imposing exactness at a set of solution nodes $X \neq Y$ leads to

$$\lambda u(x_i) - \sum_{j=1}^{|Y|} w_j k(x_i, y_j) u(y_j) = f(x_i), \quad i = 1, \ldots, |X|.$$

However, to get a closed system of equations with unknown $\hat{u} \approx u_{|X}$, we need a way to reconstruct the values $u(y_j)$ from the values $u(x_i)$.

This is clearly a scattered data approximation problem!

Decoupled Nyström method

Consider a reconstruction matrix $R \in \mathbb{R}^{|Y| \times |X|}$ such that

$$v_{|Y} \approx R\, v_{|X} \quad \text{for any } v \in C^q(\overline{\Omega}).$$

Now the decoupled system can be closed:

$$\lambda \hat{u}_i - \sum_{j=1}^{|Y|} w_j k(x_i, y_j) \sum_{\ell=1}^{|X|} (R)_{j\ell}\, \hat{u}_\ell = f(x_i).$$

In matrix notation, the linear system is simply

$$A\hat{u} := (\lambda I - KWR)\hat{u} = f_{|X},$$

with $(K)_{ij} = k(x_i, y_j)$. In general, K and R are rectangular matrices.

Refinement parameters

To properly state convergence results for the decoupled Nyström method, all the sets and matrices in its definition have to be made dependent on refinement parameters $\boldsymbol{h} = (h_X, h_Y)$:

$$A_{\boldsymbol{h}} \hat{u}_{\boldsymbol{h}} := (\lambda I_{\boldsymbol{h}} - K_{\boldsymbol{h}} W_{\boldsymbol{h}} R_{\boldsymbol{h}}) \hat{u}_{\boldsymbol{h}} = f_{|X_{\boldsymbol{h}}}.$$

$X_{\boldsymbol{h}}$ only depends on h_X, and $Y_{\boldsymbol{h}}$ only depends on h_Y. Some quantities, such as the matrices $R_{\boldsymbol{h}}$, genuinely depend on both h_X and h_Y.

For simplicity, let us assume from now on that

$$h_X = C_X h \quad \text{and} \quad h_Y = C_Y h$$

for some constants $C_X, C_Y > 0$ and a single scalar parameter $h > 0$.

Error analysis of decoupled Nyström method

Proposition

Consider the decoupled Nyström method for $(\lambda I - \mathcal{K})u = f$. If

1. $f \in C^q(\overline{\Omega})$, $k \in C^q(\overline{\Omega} \times \overline{\Omega})$, $\lambda \notin \sigma(\mathcal{K})$.
2. The quadrature scheme $(Y_{\boldsymbol{h}}, w_{\boldsymbol{h}})$ is stable with respect to the vector 1-norm, and has convergence order $q_W \leq q$.
3. The reconstruction scheme $(X_{\boldsymbol{h}}, Y_{\boldsymbol{h}}, R_{\boldsymbol{h}})$ is stable with respect to the matrix ∞-norm, and has convergence order $q_R \leq q$.

Then, for small $\boldsymbol{h} > 0$, the linear system $A_{\boldsymbol{h}} \hat{u}_{\boldsymbol{h}} = f_{|X_{\boldsymbol{h}}}$ has a unique solution, $\kappa_\infty(A_{\boldsymbol{h}})$ is bounded, and there exist $C_1, C_2 > 0$ such that

$$\left\| u_{|X_{\boldsymbol{h}}} - \hat{u}_{\boldsymbol{h}} \right\|_\infty \leq C_1 h_Y^{q_W} \left\| \| k(x,y) \|_{C^q(\overline{\Omega}),y} \right\|_{\infty,x} \|u\|_{C^q(\overline{\Omega})}$$

$$+ C_2 h_X^{q_R} \|k\|_{C^0(\overline{\Omega}\times\overline{\Omega})} \|u\|_{C^q(\overline{\Omega})} .$$

Error analysis of decoupled Nyström method

Sketch of the proof

The proof is adapted from Section 4.1 of Atkinson's monograph *The Numerical Solution of Integral Equations of the Second Kind* and relies on the framework of collectively compact operator approximations.

Define the family of linear operators $\mathcal{K}_{\boldsymbol{h}} \colon C^q(\overline{\Omega}) \to C^q(\overline{\Omega})$ by

$$(\mathcal{K}_{\boldsymbol{h}} u)(x) = k(x, Y_{\boldsymbol{h}}) W_{\boldsymbol{h}} R_{\boldsymbol{h}} u_{|X_{\boldsymbol{h}}},$$

with $k(x, Y_{\boldsymbol{h}})$ being the row vector of values $\{k(x, y_{\boldsymbol{h},j}) \mid y_{\boldsymbol{h},j} \in Y_{\boldsymbol{h}}\}$.

We have shown that $\{\mathcal{K}_{\boldsymbol{h}}\}$ is a collectively compact family of pointwise convergent operators. Then the error estimate follows from Theorem 4.1.1 and Lemma 4.1.2 in Atkinson's book, after some calculations.

Decoupled Nyström in a meshless setting

Meshless methods

Meshless (aka meshfree) methods are a versatile class of numerical techniques that discretize computational domains using scattered, unstructured nodes, avoiding the complexities and limitations of conventional mesh generation.

To solve Fredholm's integral equations and experiment with the decoupled Nyström method, we have placed quasi-uniform scattered nodes in the interior of Ω using the advancing front algorithm in the library `https://github.com/BrunoDegliEsposti/NodeGenLib`

The C++ library has a MATLAB interface, supports 2D/3D domains, and even trimmed CAD geometries for real-world applications.

Example of boundary nodes produced by NodeGenLib in 3D

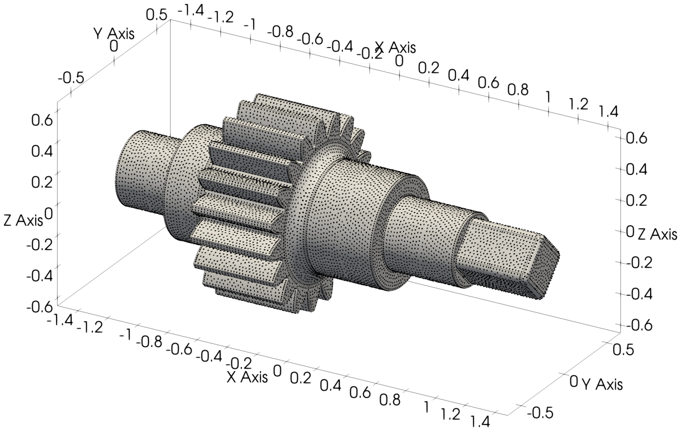


Figure: NodeGenLib boundary nodes on gear shaft for $h = 0.02$.

Example of interior nodes produced by NodeGenLib in 3D

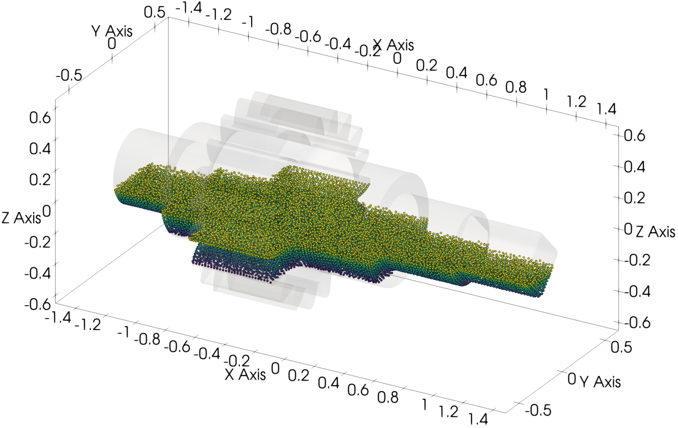


Figure: NodeGenLib interior nodes on gear shaft for $h = 0.02$.

Meshless moment-free quadrature formulas

Quadrature formulas on scattered data are found using a recently developed meshless approach that requires neither meshing nor moment computation [1]. Stable quadrature weights are found as a minimum-norm solution to a sparse linear system obtained as a discretization of the divergence theorem by numerical differentiation formulas, such as those used in polyharmonic RBF-FD.

Sparse interpolation matrices $R_{\boldsymbol{h}}$ are computed using local polyharmonic RBF interpolation with polynomial augmentation of order q_R, as implemented in the library `mFDlab` by Oleg Davydov.

A new result on the stability of $R_{\boldsymbol{h}}$ for local polyharmonic RBF interpolation was presented by Oleg on Monday.

[1] Oleg Davydov and Bruno Degli Esposti (2025). *Meshless moment-free quadrature formulas arising from numerical differentiation*, CMAME.

Numerical experiments

Kernels and numerical errors

For the numerical experiments we use normalized Gaussian kernels

$$k(x,y) = (\sigma\sqrt{2\pi})^{-d}\exp\left(-\|x-y\|^2/(2\sigma^2)\right)$$

with $d = 2$ and standard deviation $\sigma > 0$.

Relative numerical errors are computed in the L^2 norm by integrating the squared error with $(Y_{\boldsymbol{h}}, w_{\boldsymbol{h}})$. The squared error is smooth by the Nyström interpolation formula.

To evaluate numerical errors, the source term f is chosen so that u is a known function (manufactured solution). In these tests, u is Franke's function remapped from $[0,1]^2$ to $[-1,1]^2$.

The dense linear system $A_{\boldsymbol{h}}\hat{u}_{\boldsymbol{h}} = f_{|X_{\boldsymbol{h}}}$ is solved with a direct method.

Choice of domain and nodes

Let Ω be the region enclosed by a Cassini oval, a quartic plane curve defined as the locus of points such that the product of the distances to two fixed points $(-a, 0)$ and $(a, 0)$ is a constant $b^2 \in \mathbb{R}_+$:

$$\Omega = \left\{ (x_1, x_2) \in \mathbb{R}^2 \;\middle|\; \left((x_1 + a)^2 + x_2^2\right)\left((x_1 - a)^2 + x_2^2\right) - b^4 < 0 \right\}.$$

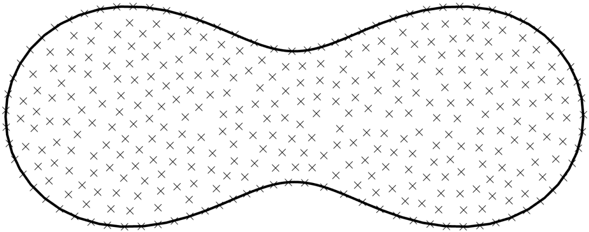


Figure: Cassini oval with $a = 0.95$ and $b = 1$. Scattered nodes generated by NodeGenLib with spacing parameter $h = 0.05$.

Convergence orders

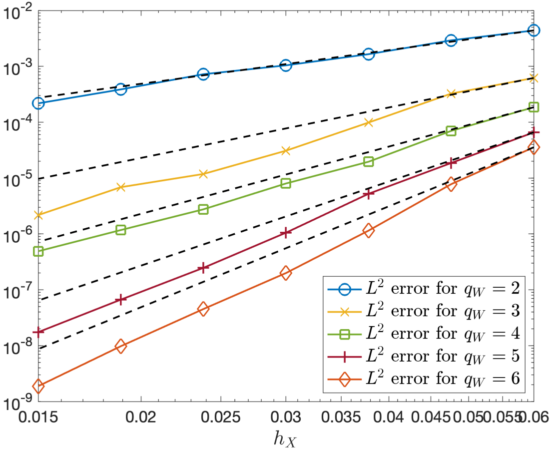


Figure: Relative numerical errors as functions of h_X for different orders q_W. $h_Y = h_X/2$, $\lambda = 1$, $q_R = q_W$, Gaussian kernel with $\sigma = 0.1$.

Efficiency test with localized Gaussian kernel

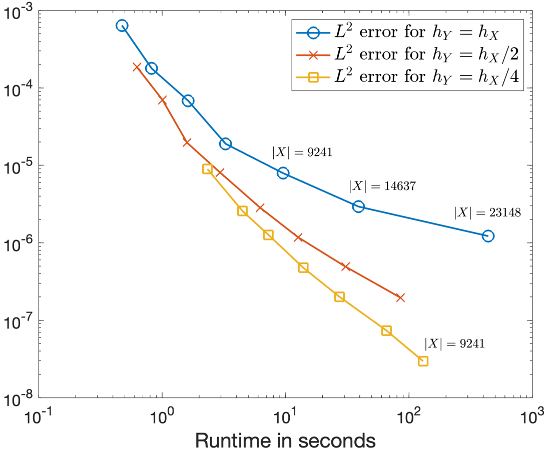


Figure: Numerical errors as functions of runtime for different ratios h_X/h_Y. $\lambda = 1$, $q_W = 5$, $q_R = 5$, Gaussian kernel with $\sigma = 0.1$.

Nonlinear population dynamics model

Motivated by nonlocal models for population dynamics widely used in ecology, we seek to compute equilibrium states of

$$u_t = \int_\Omega k(x,y)\big(u(y) - u(x)\big)\, dy + u(x)\big(a(x) - u(x)\big),$$

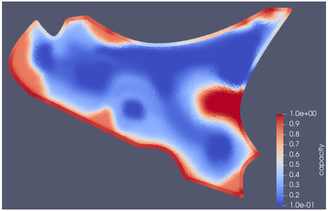
i.e. a nonlinear Fredholm integro-differential equation with

- Homogeneous Neumann boundary conditions
- Logistic growth with carrying capacity $a(x)$

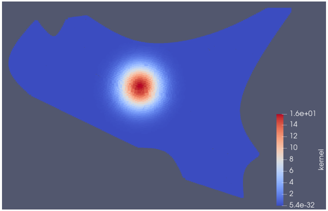
The nonlinear system is solved using Newton's method with $u^{(0)} = a$.

We choose a domain Ω whose shape resembles the island of Sicily, with piecewise cubic C^0 boundary. The carrying capacity $a(x)$ is a smoothed height map computed from elevation data.

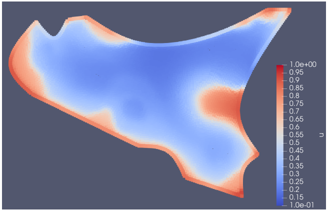
Nonlinear population dynamics model



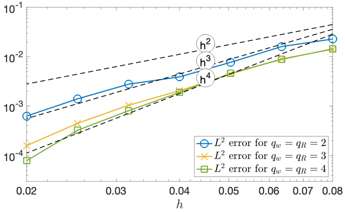
(a) Carrying capacity $a(x)$.



(b) Gaussian kernel $k(0, y)$.



(c) Numerical solution.



(d) Error convergence plot.

Conclusion and future work

Conclusion

Solution nodes X can be decoupled from quadrature nodes Y in Nyström's method. Theoretical analysis and numerical experiments demonstrate significantly better efficiency for localized kernels.

Directions for future work

- Compression of A using ACA.
  How does it affect the optimal ratio h_X/h_Y?
- Extension to evolution equations
- Extension to 3D domains and surfaces
- Extension to singular/near-singular kernels by locally refining Y
- Decoupled Nyström method to find eigenvalues of $\mathcal{K}$

Conclusion and future work

Thank you for your attention!

And once again, happy birthday Alessandra!
Thank you for everything that you've taught me over the last 5+ years.

Extra slides

Manufactured solutions with Chebfun

Compared to PDEs, the method of manufactured solutions is harder to apply to integral equations, because we cannot easily evaluate the integral over Ω in the expression that defines the right-hand side

$$f(x_i) := \lambda u(x_i) - \int_\Omega k(x_i, y) u(y)\, dy, \quad x_i \in X.$$

We propose the following new approach for all $x_i \in X$:

- Approximate the function $y \mapsto k(x_i, y)u(y)$ to machine precision with a bivariate polynomial $p_i(y)$ over a bounding box around Ω using the open-source library Chebfun.
- Find polynomial field F_i such that $\mathrm{div}(F_i)(y) = p_i(y)$ exactly.
- Evaluate the integral over Ω up to machine precision using the divergence theorem and adaptive Gaussian quadrature on each smooth piece of $\partial\Omega$, assuming that parametrizations are known.