Introduction to Numerical Differential Equations

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Some examples of differential equations

- A one-dimensional differential equation

$$
\begin{gathered}
\big(a(x)u'\big)' + \kappa^2(x)u = f(x), \quad x \in \Omega := (0,1) \\
\lambda_0^L u(0) + \lambda_1^L u'(0) = g_0,\ \lambda_0^R u(1) + \lambda_1^R u'(1) = g_1.
\end{gathered}
$$

- The 2D Poisson equation with a variable coefficient

$$
\begin{aligned}
-\nabla \cdot (a(x)\nabla u(x)) &= f(x), && x \in \Omega := (0,1)^2, \\
u(x) &= 0, && x \in \partial\Omega.
\end{aligned}
$$

- The 2D Helmholtz equation

$$
\begin{aligned}
-\Delta u - \kappa^2 u &= f, \quad \text{in } \Omega := (0,1)^2, \\
\frac{\partial u}{\partial \nu} - \mathrm{i}\kappa u &= g, \quad \text{on } \partial\Omega.
\end{aligned}
$$

Some examples of differential equations

- The 1D heat equation

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= k\frac{\partial^2 u(x,t)}{\partial x^2}, && x \in (0,L),\ t>0,\\
u(0,t) &= u(L,t) = 0, && t>0,\\
u(x,0) &= f(x), && x \in (0,L).
\end{aligned}
$$

- The 1D wave equation

$$
\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial t^2} &= a^2\frac{\partial^2 u(x,t)}{\partial x^2}, && x \in (0,L),\ t>0,\\
u(0,t) &= u(L,t) = 0, && t>0,\\
u(x,0) &= f(x), && x \in (0,L),\\
u_t(x,0) &= g(x), && x \in (0,L),
\end{aligned}
$$

Outline of today's lecture

- Finite difference method
- Wavelet Galerkin method
- Physics-informed neural network
- Neural operator

A simple example of 1D FDM

Consider the following 1D Poisson equation

$$-u'' = f \text{ in } (0,1), \quad u(0) = u(1) = 0.$$

Let $x_j = j/N$, where $j = 0, \ldots, N$, $x_0 := 0$, and $x_N := 1$, be a uniform grid that partitions $[0,1]$ with a grid size $h = 1/N$. By Taylor expansions,

$$-u''(x_j) = \frac{-1u(x_{j+1}) + 2u(x_j) - 1u(x_{j-1})}{h^2} + \mathcal{O}(h^2), \quad h \to 0.$$

To find the approximated value for $u(x_j)$, denoted by u_j, we need to solve

$$\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = h^2 \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \\ f(x_{N-2}) \\ f(x_{N-1}) \end{bmatrix}.$$

A simple example of 2D FDM

The 2D Poisson equation with a variable coefficient

$$
\begin{aligned}
-\nabla \cdot (a(x)\nabla u(x)) &= f(x), && x \in \Omega := (0,1)^2,\\
u(x) &= 0, && x \in \partial\Omega.
\end{aligned}
$$

Let $(x_i, y_j) = (i/N, j/N)$, where $i, j = 0, \ldots, N$, $x_0 = y_0 = 0$, and $x_N = y_N = 1$, be a uniform grid that partitions $[0,1]^2$ with a grid size $h = 1/N$ for each axis.

Let $u_{i,j}$ denote the approximated value for $u(x_i, y_j)$. A second-order finite difference scheme reads

$$
\begin{aligned}
-a_{i-1/2,j}u_{i-1,j} - a_{i,j-1/2}u_{i,j-1} - a_{i+1/2,j}u_{i+1,j} - a_{i,j+1/2}u_{i,j+1}\\
+(a_{i+1/2,j} + a_{i-1/2,j} + a_{i,j+1/2} + a_{i,j-1/2})u_{i,j} = h^2 f(x_i, y_j),
\end{aligned}
$$

where $a_{i+1/2,j} = \frac{1}{2}(a_{i+1,j} + a_{i,j})$, $a_{i-1/2,j} = \frac{1}{2}(a_{i,j} + a_{i-1,j})$, and $a_{i,j+1/2}$, $a_{i,j-1/2}$ are defined similarly.

The linear system has a block triadiagonal structure. Let's do a demo.

1D model problem

Consider the following 1D heterogeneous Helmholtz equation

$$\begin{aligned}
\mathcal{L}u &:= \big(a(x)u'\big)' + \kappa^2(x)u = f(x), \quad x \in \Omega := (0,1)\\
\mathcal{B}_0 u(0) &:= \lambda_0^L u(0) + \lambda_1^L u'(0) = g_0,\\
\mathcal{B}_1 u(1) &:= \lambda_0^R u(1) + \lambda_1^R u'(1) = g_1,
\end{aligned}$$

where $f \in L_2(\Omega)$ and $a(x), \kappa(x)$ are bounded piecewise smooth functions such that $\operatorname{ess-inf}_{x\in\Omega} a(x) > 0$.

Arbitrarily accurate 1D compact FDM

Propn Suppose a, κ^2, f, u are analytic functions satisfying the model problem for all $x \in (0,1)$.

For any point $x_b \in (0,1)$, we have

$$u^{(j)}(x_b) = E_{j,0}u(x_b) + E_{j,1}u'(x_b) + \sum_{\ell=0}^{j-2} F_{j,\ell} f^{(\ell)}(x_b), \qquad j \geqslant 2,$$

where $E_{j,0}, E_{j,1}, F_{j,\ell}$ only depend on $a(x_b), a'(x_b), \ldots, a^{(j-1)}(x_b)$ and $\kappa^2(x_b)$, $[\kappa^2]'(x_b), \ldots, [\kappa^2]^{(j-2)}(x_b)$ for $j \geqslant 2$ and $\ell \in \mathbb{N}_0$.

For sufficiently small h,

$$u(x_b + h) = u(x_b)E_0(h) + u'(x_b)hE_1(h) + \sum_{\ell=0}^{\infty} h^{\ell+2} f^{(\ell)}(x_b) F_\ell(h) \quad \text{with}$$

$$E_0(h) := 1 + \sum_{j=2}^{\infty} \frac{E_{j,0}}{j!} h^j, \; E_1(h) := 1 + \sum_{j=2}^{\infty} \frac{E_{j,1}}{j!} h^{j-1}, \; F_\ell(h) := \sum_{j=\ell+2}^{\infty} \frac{F_{j,\ell}}{j!} h^{j-\ell-2}.$$

Thm Suppose a, κ^2, f are smooth functions. Let $M, \tilde{M} \in \mathbb{N}$ with $M \geqslant \tilde{M}$, $0 < h < 1$, and $x_b \in (0,1)$ such that $(x_b - h, x_b + h) \subset (0,1)$. Then, for every solution u of $\mathcal{L}u = f$,

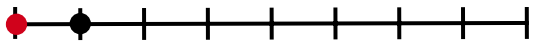
$$\frac{c_{-1}(h)u(x_b - h) + c_0(h)u(x_b) + c_1(h)u(x_b + h)}{h^2} - \sum_{\ell=0}^{\tilde{M}-1} d_\ell(h) h^\ell f^{(\ell)}(x_b) = \mathcal{O}(h^{\tilde{M}}),$$

where $h \to 0$ and for $\ell = 0, \ldots, \tilde{M} - 1$,

$$c_1(h) = \frac{\alpha(h)}{E_1(h)} + \mathcal{O}(h^{M+1}), \quad c_{-1}(h) = \frac{\alpha(h)}{E_1(-h)} + \mathcal{O}(h^{M+1}),$$
$$c_0(h) = -c_1(h)E_0(h) - c_{-1}(h)E_0(-h) + \mathcal{O}(h^{M+2}),$$
$$d_\ell(h) = c_1(h)F_\ell(h) + (-1)^\ell c_{-1}(h)F_\ell(-h) + \mathcal{O}(h^{\tilde{M}-\ell}), \quad h \to 0,$$

and α is smooth with $\alpha(0) \neq 0$.

Arbitrarily accurate 1D compact FDM



Thm Suppose a, κ^2, f are smooth. Let $M, \tilde{M} \in \mathbb{N}$ with $M \geqslant \tilde{M}$, $0 < h < 1$, and $x_b \in [0,1)$ with $(x_b, x_b + h) \subset (0,1)$. Define

$$\mathcal{B}^+ u(x_b) := \lambda_0 u(x_b+) + \lambda_1 u'(x_b+) \quad \text{with} \quad \lambda_0, \lambda_1 \in \mathbb{C}.$$

Then, for every solution u of $\mathcal{L}u = 0$,

$$\frac{c_0^{\mathcal{B}^+}(h)u(x_b) + c_1^{\mathcal{B}^+}(h)u(x_b+h)}{h} - \sum_{\ell=0}^{\tilde{M}-2} d_\ell^{\mathcal{B}^+}(h) h^{\ell+1} f^{(\ell)}(x_b+) - \mathcal{B}^+ u(x_b) = \lambda(h^{\tilde{M}}),$$

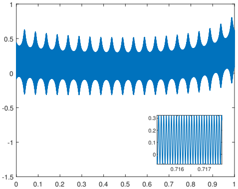
where $h \to 0$ and

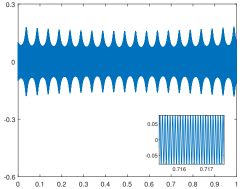
$$c_1^{\mathcal{B}^+}(h) = \frac{\lambda_1}{E_1(h)} + \mathcal{O}(h^M), \quad c_0^{\mathcal{B}^+}(h) = h\lambda_0 - c_1^{\mathcal{B}^+}(h)E_0(h) + \mathcal{O}(h^{M+1}),$$

$$d_\ell^{\mathcal{B}^+}(h) = c_1^{\mathcal{B}^+}(h) F_\ell(h) + \mathcal{O}(h^{\tilde{M}-\ell-1}), \quad \ell = 0, \dots, \tilde{M}-2, \quad h \to 0.$$

Example

Consider the model problem with $a = 1.1 + \sin(40\pi x)$, $\kappa = 10^5\left(1 - (x-0.5)^2\right)$, $f = 10^9(x^7+1)$, and the boundary conditions $\sqrt{1.1}u'(0) + i75000u(0) = -1$ and $\sqrt{1.1}u'(1) - i75000u(1) = 0$.





		DAT using the compact FDM with order $M=6$				DAT using the compact FDM with order $M=8$			
N	ℓ	$\frac{\|u_N-u_{2N-1}\|_\infty}{\|u_{2N-1}\|_\infty}$	$\frac{\|u'_N-u'_{2N-1}\|_\infty}{\|u'_{2N-1}\|_\infty}$	Local CN	Link CN	$\frac{\|u_N-u_{2N-1}\|_\infty}{\|u_{2N-1}\|_\infty}$	$\frac{\|u'_N-u'_{2N-1}\|_\infty}{\|u'_{2N-1}\|_\infty}$	Local CN	Link CN
$2^{18}+1$	0	4.8707×10^{-1}	7.6812×10^{-1}	5.53×10^{6}	–	6.7606×10^{-3}	1.0602×10^{-2}	5.66×10^{6}	–
	16	4.8707×10^{-1}	7.6812×10^{-1}	2.74×10^{5}	7.71×10^{6}	6.7606×10^{-3}	1.0602×10^{-2}	5.25×10^{5}	1.20×10^{7}
$2^{19}+1$	0	7.1208×10^{-3}	1.1068×10^{-2}	1.47×10^{7}	–	2.2709×10^{-5}	3.5577×10^{-5}	1.42×10^{7}	–
	17	7.1208×10^{-3}	1.1068×10^{-2}	4.39×10^{1}	1.16×10^{7}	2.2709×10^{-5}	3.5577×10^{-5}	4.39×10^{1}	1.19×10^{7}
$2^{20}+1$	0	1.0754×10^{-4}	1.6712×10^{-4}	6.21×10^{7}	–	8.6824×10^{-8}	1.3591×10^{-7}	5.98×10^{7}	–
	18	1.0754×10^{-4}	1.6712×10^{-4}	4.47×10^{1}	1.19×10^{7}	8.6814×10^{-8}	1.3589×10^{-7}	4.47×10^{1}	1.19×10^{7}
$2^{21}+1$	0	1.6652×10^{-6}	2.5876×10^{-6}	2.23×10^{8}	–	1.9291×10^{-9}	2.9177×10^{-9}	2.23×10^{8}	–
	19	1.6652×10^{-6}	2.5877×10^{-6}	4.49×10^{1}	1.19×10^{7}	1.8549×10^{-9}	2.8085×10^{-9}	4.49×10^{1}	1.19×10^{7}

2D model problem

Let $\Omega := (l_1, l_2) \times (l_3, l_4)$ and ψ be a smooth two-dimensional function. Consider a smooth curve $\Gamma_I := \{(x, y) \in \Omega : \psi(x, y) = 0\}$, which partitions Ω into

$$\Omega^+ := \{(x, y) \in \Omega \ : \ \psi(x, y) > 0\} \quad \text{and} \quad \Omega^- := \{(x, y) \in \Omega \ : \ \psi(x, y) < 0\}.$$

Our model problem is

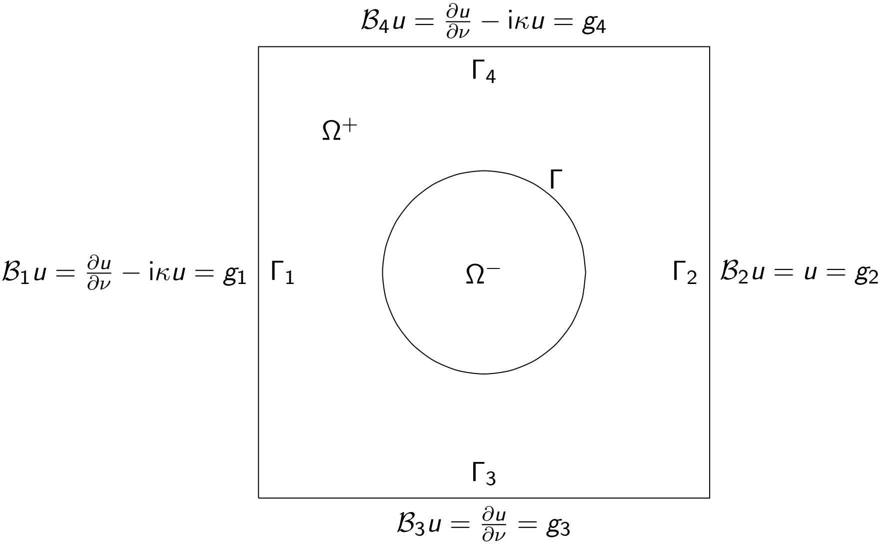
$$\begin{cases} \Delta u + \kappa^2 u = f & \text{in } \Omega \setminus \Gamma, \\ [u] = g_D, \quad [\nabla u \cdot \nu] = g_N & \text{on } \Gamma, \\ \mathcal{B}_1 u = g_1 \text{ on } \Gamma_1 := \{l_1\} \times (l_3, l_4), & \mathcal{B}_2 u = g_2 \text{ on } \Gamma_2 := \{l_2\} \times (l_3, l_4), \\ \mathcal{B}_3 u = g_3 \text{ on } \Gamma_3 := (l_1, l_2) \times \{l_3\}, & \mathcal{B}_4 u = g_4 \text{ on } \Gamma_4 := (l_1, l_2) \times \{l_4\}, \end{cases}$$

where $\mathcal{B}_j \in \{\mathbf{I}_d$ (Dirichlet), $\frac{\partial}{\partial \nu}$ (Neumann), $\frac{\partial}{\partial \nu} - \mathrm{i}\kappa \mathbf{I}_d$ (radiation)$\}$ and for any point $(x_0, y_0) \in \Gamma$,

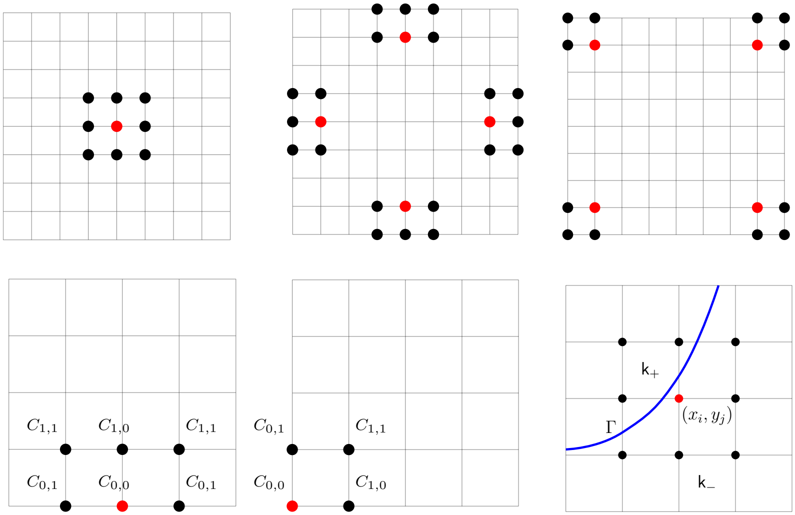
$$[u](x_0, y_0) := \lim_{\substack{(x,y) \in \Omega^+, \\ (x,y) \to (x_0, y_0)}} u(x, y) - \lim_{\substack{(x,y) \in \Omega^-, \\ (x,y) \to (x_0, y_0)}} u(x, y),$$

$$[\nabla u \cdot \nu](x_0, y_0) := \lim_{\substack{(x,y) \in \Omega^+, \\ (x,y) \to (x_0, y_0)}} \nabla u(x, y) \cdot \nu - \lim_{\substack{(x,y) \in \Omega^-, \\ (x,y) \to (x_0, y_0)}} \nabla u(x, y) \cdot \nu.$$

2D model problem



Construction of interior, edge, and corner stencils

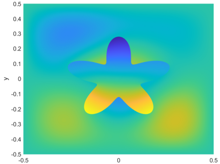


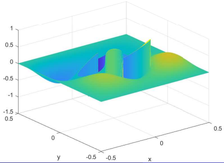
Example

Suppose $\Omega = (-1/2, 1/2)^2$ with $(\kappa_+, \kappa_-) \in \{(10,1), (1,100)\}$, the source term is $f_+ = \sin(2\pi x)\sin(2\pi y)$, $f_- = \cos(2\pi x)\cos(2\pi y)$, and the boundary conditions are

$$
\begin{aligned}
&g = \sin(\theta), \qquad g_\Gamma = \cos(\theta), \quad \text{for} \quad \theta \in [0, 2\pi), \\
&u(-1/2, y) = 0, \quad \text{and} \quad u(1/2, y) = 0 \quad \text{for} \quad y \in (-1/2, 1/2), \\
&u(x, -1/2) = 0, \quad \text{and} \quad u(x, 1/2) = 0 \quad \text{for} \quad x \in (-1/2, 1/2).
\end{aligned}
$$

$\kappa_+ = 10$ and $\kappa_- = 1$						$\kappa_+ = 1$ and $\kappa_- = 100$					
J	$\frac{2\pi}{h\kappa_+}$	$\Vert u_h - u_{h/2}\Vert_2$	order	$\Vert u_h - u_{h/2}\Vert_\infty$	order	J	$\frac{2\pi}{h\kappa_-}$	$\Vert u_h - u_{h/2}\Vert_2$	order	$\Vert u_h - u_{h/2}\Vert_\infty$	order
6	40.2	8.2461E-01		3.6325E+00							
7	80.4	8.0665E-03	6.7	4.4579E-02	6.3	7	8.0	3.5212E-02		2.6626E-01	
8	160.8	9.3400E-05	6.4	6.5308E-04	6.1	8	16.1	9.6191E-04	5.2	6.9248E-03	5.3
9	321.7	3.0871E-06	4.9	2.2701E-05	4.8	9	32.2	2.4508E-05	5.3	1.5983E-04	5.4
10	643.4	1.9575E-08	7.3	2.2072E-07	6.7	10	64.3	8.0117E-07	4.9	5.2179E-06	4.9



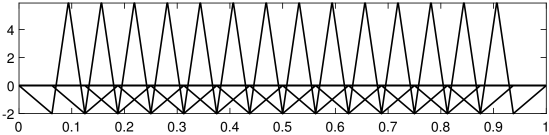


Preliminaries on wavelets

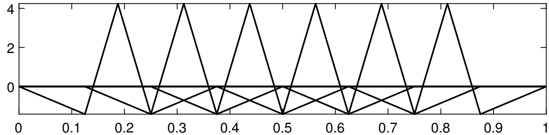
Let $\phi := (\phi^1, \ldots, \phi^r)^\mathsf{T}$ and $\psi := (\psi^1, \ldots, \psi^s)^\mathsf{T}$ be vectors of functions in $L_2(\mathbb{R})$. For $J \in \mathbb{Z}$, a wavelet system $\mathcal{B}_{J_0}(\phi; \psi)$ is defined to be

$$\mathcal{B}_{J_0}(\phi;\psi) := \{\phi^\ell_{J_0;k} \ : \ k \in \mathbb{Z}, \ell = 1, \ldots, r\} \cup \{\psi^\ell_{j;k} \ : \ j \geqslant J_0, k \in \mathbb{Z}, \ell = 1, \ldots, s\},$$

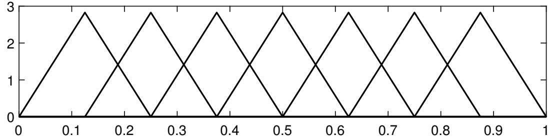
where $\phi^\ell_{J_0;k} := 2^{J_0/2}\phi^\ell(2^{J_0} \cdot -k)$ and $\psi^\ell_{j;k} := 2^{j/2}\psi^\ell(2^j \cdot -k)$.



$\{2^2\psi(2^4 \cdot -k), k = 1, \ldots, 14\}$



$\{2^{3/2}\psi(2^3 \cdot -k), k = 1, \ldots, 6\}$



$\{2^{3/2}\phi(2^3 \cdot -k), k = 1, \ldots, 7\}$

Preliminaries on wavelets

We say that $\mathcal{B}_{J_0}(\phi;\psi)$ is a Riesz basis of $L_2(\mathbb{R})$ if the linear span of $\mathcal{B}_{J_0}(\phi;\psi)$ is dense in $L_2(\mathbb{R})$ and $\mathcal{B}_{J_0}(\phi;\psi)$ is a Riesz sequence in $L_2(\mathbb{R})$, i.e., there exist positive constants C_1 and C_2 such that

$$C_1 \sum_{h\in\mathcal{B}_{J_0}(\phi;\psi)} |c_h|^2 \leqslant \Big\| \sum_{h\in\mathcal{B}_{J_0}(\phi;\psi)} c_h h \Big\|_{L_2(\mathbb{R})}^2 \leqslant C_2 \sum_{h\in\mathcal{B}_{J_0}(\phi;\psi)} |c_h|^2$$

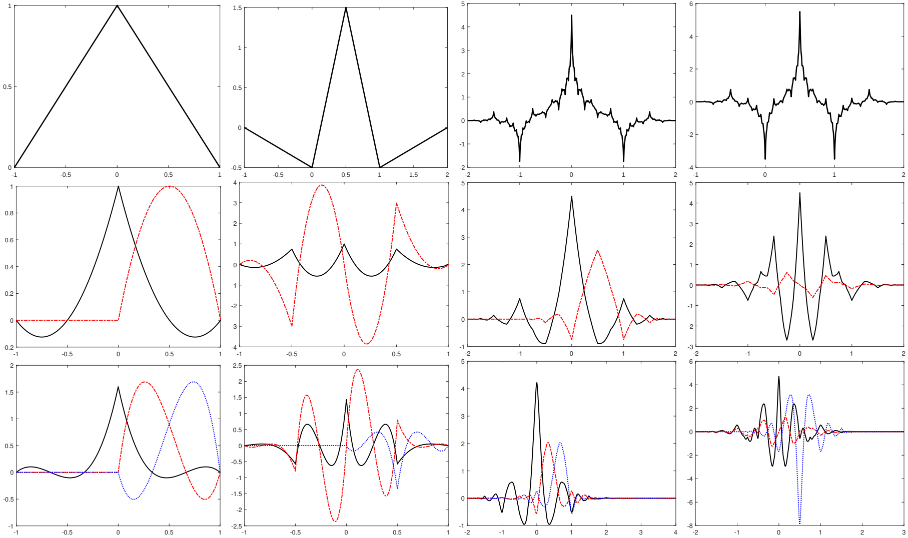
for all finitely supported sequences $\{c_h\}_{h\in\mathcal{B}_{J_0}(\phi;\psi)}$.

We say that $\{\phi;\psi\}$ is a Riesz wavelet in $L_2(\mathbb{R})$ if $\mathcal{B}_{J_0}(\phi;\psi)$ is a Riesz basis of $L_2(\mathbb{R})$.

Let $\tilde{\phi} := (\tilde{\phi}^1,\dots,\tilde{\phi}^r)^\mathsf{T}$ and $\tilde{\psi} := (\tilde{\psi}^1,\dots,\tilde{\psi}^s)^\mathsf{T}$ be vectors of functions in $L_2(\mathbb{R})$. We say that $(\{\tilde{\phi};\tilde{\psi}\},\{\phi;\psi\})$ is a biorthogonal wavelet in $L_2(\mathbb{R})$ if both $\{\tilde{\phi};\tilde{\psi}\}$ and $\{\phi;\psi\}$ are Riesz bases in $L_2(\mathbb{R})$ such that $\mathcal{B}_{J_0}(\tilde{\phi};\tilde{\psi})$ and $\mathcal{B}_{J_0}(\phi;\psi)$ are biorthogonal to each other in $L_2(\mathbb{R})$.

Three examples of biorthogonal wavelets

Left to right: $\phi, \psi, \tilde{\phi}$, and $\tilde{\psi}$. Each row represents an example.



Fundamental result on biorthogonal wavelets

Thm: Let $\phi, \tilde{\phi}$ be $r \times 1$ vectors of compactly supported distributions and $\psi, \tilde{\psi}$ be $s \times 1$ vectors of compactly supported distributions on $\mathbb{R}$. Then $(\{\tilde{\phi}; \tilde{\psi}\}, \{\phi; \psi\})$ is a biorthogonal wavelet in $L_2(\mathbb{R})$ iff

(1) $\phi, \tilde{\phi} \in (L_2(\mathbb{R}))^r$ and $\overline{\widehat{\phi}(0)}^{\mathsf{T}} \widehat{\tilde{\phi}}(0) = 1$.

(2) ϕ and $\tilde{\phi}$ are biorthogonal to each other: $\langle \phi, \tilde{\phi}(\cdot - k) \rangle = \boldsymbol{\delta}(k) I_r$ for all $k \in \mathbb{Z}$.

(3) There exist $a, \tilde{a}, b, \tilde{b} \in (l_0(\mathbb{Z}))^{r \times r}$ (finitely supported sequences)

$$\phi = 2 \sum_{k \in \mathbb{Z}} a(k) \phi(2 \cdot - k), \qquad \psi = 2 \sum_{k \in \mathbb{Z}} b(k) \phi(2 \cdot - k),$$

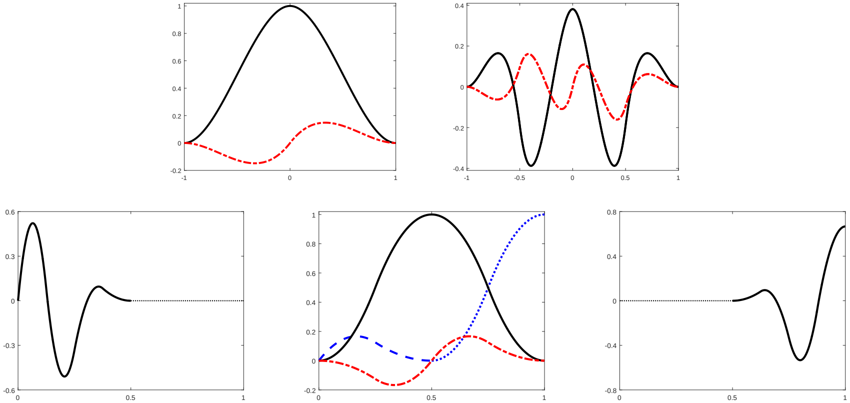
$$\tilde{\phi} = 2 \sum_{k \in \mathbb{Z}} \tilde{a}(k) \tilde{\phi}(2 \cdot - k), \qquad \tilde{\psi} = 2 \sum_{k \in \mathbb{Z}} \tilde{b}(k) \tilde{\phi}(2 \cdot - k),$$

and $(\{\tilde{a}; \tilde{b}\}, \{a; b\})$ is a biorthogonal wavelet filter bank, i.e., $s = r$ and

$$\begin{bmatrix} \widehat{\tilde{a}}(\xi) & \widehat{\tilde{a}}(\xi + \pi) \\ \widehat{\tilde{b}}(\xi) & \widehat{\tilde{b}}(\xi + \pi) \end{bmatrix} \begin{bmatrix} \overline{\widehat{a}(\xi)}^{\mathsf{T}} & \overline{\widehat{b}(\xi)}^{\mathsf{T}} \\ \overline{\widehat{a}(\xi + \pi)}^{\mathsf{T}} & \overline{\widehat{b}(\xi + \pi)}^{\mathsf{T}} \end{bmatrix} = I_{2r}, \qquad \xi \in \mathbb{R}.$$

(4) Every element in ψ and $\tilde{\psi}$ has at least one vanishing moment.

One more example of a wavelet system



Define $\Phi_1 := \{\phi^L_{1;0}, \phi_{1;1}, \phi^R_{1;1}\}$,

$$\Psi_j := \{\psi^L_{j;0}\} \cup \{\psi_{j;k} \ : \ 1 \leqslant k \leqslant 2^j - 1\} \cup \{\psi^R_{j;2^j-1}\}, \quad j \geqslant J_0, \quad \text{and}$$

$$\mathcal{B}^{1\mathrm{D}}_{1,J} := \Phi_1 \cup \cup_{j=J_0}^{J-1} \Psi_j.$$

Example

Consider the following differential equation:

$$-u'' + 5u = f \text{ on } (0,1), \quad u(0) = 0, \quad u'(1) = 0,$$

where the exact solution is $u(x) = 100(1 - e^{-x}) - 100e^{-1}x$. Let

$$u_J := \sum_{\eta \in \mathcal{B}_{1,J}^{1\mathrm{D}}} c_\eta \eta.$$

The coefficients c_η can be found by solving the following linear system

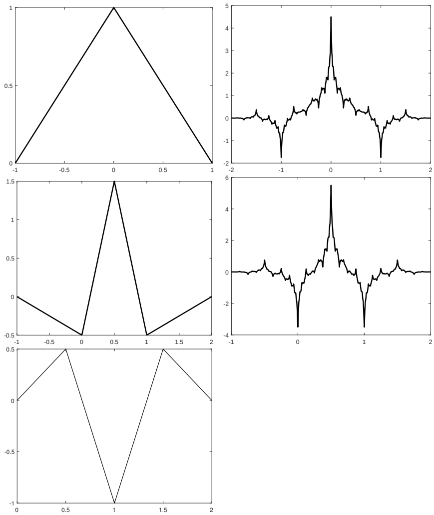
$$\langle u_J', v\rangle + \langle u_J, v\rangle = \langle f, v\rangle, \quad v \in \mathcal{B}_{1,J}^{1\mathrm{D}}.$$

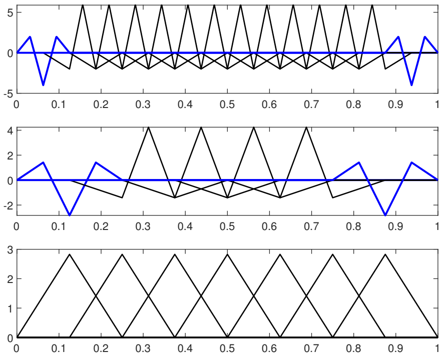
Level	Size	Iteration	κ	$\|e_n\|_{L_\infty}$	$\|e_n\|_{L_2}$	$\log_2 \frac{\|e_{n-1}\|_{L_2}}{\|e_n\|_{L_2}}$
5	128	15	3.2106	4.2213e-07	1.8141e-07	3.0089
6	256	15	3.2106	5.2757e-08	2.2607e-08	3.0044
7	512	15	3.2106	6.5948e-09	2.8215e-09	3.0022
8	1024	15	3.2106	8.2152e-10	3.5243e-10	3.0011
9	2048	16	3.2106	1.1396e-10	4.5919e-11	2.9402

How about the 2D case?

- Any compactly supported biorthogonal wavelet can be adapted to the unit interval.
- Use tensor product.
- Use the weak formulation to obtain an approximated solution.

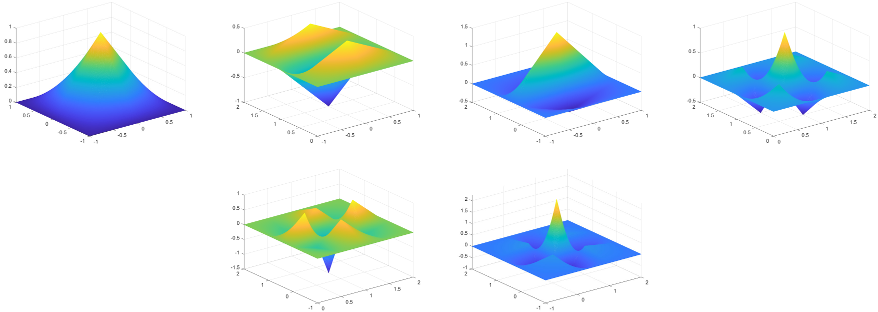
Biorthogonal wavelet in $H_0^1(\Omega)$ from the 2D hat function





Biorthogonal wavelet in $H_0^1(\Omega)$ from the 2D hat function

Below are plots of some generators of $\mathcal{B}_{J_0}^{H_0^1(\Omega)}$:



Wavelets in $L_2(\mathcal{I})$, $\mathcal{I} := (0,1)$.

Given a compactly supported biorthogonal wavelet $(\{\tilde{\phi};\tilde{\psi}\},\{\phi;\psi\})$ in $L_2(\mathbb{R})$, we construct a biorthogonal wavelet $(\tilde{\mathcal{B}}^{1\mathrm{D}},\mathcal{B}^{1\mathrm{D}})$ in $L_2(\mathcal{I})$

$$\mathcal{B}^{1\mathrm{D}}_{J_0} := \Phi_{J_0} \cup \cup_{j=J_0}^{\infty} \Psi_j \subseteq L_2(\mathcal{I}), \qquad \tilde{\mathcal{B}}^{1\mathrm{D}}_{J_0} := \tilde{\Phi}_{J_0} \cup \cup_{j=J_0}^{\infty} \tilde{\Psi}_j \subseteq L_2(\mathcal{I}),$$

where $J_0 \in \mathbb{N}$,

$$\Phi_{J_0} = \{\phi^L_{J_0;0}\} \cup \{\phi_{J_0;k} \ : \ n_{l,\phi} \leqslant k \leqslant 2^{J_0} - n_{h,\phi}\} \cup \{\phi^R_{J_0;2^{J_0}-1}\},$$
$$\Psi_j = \{\psi^L_{j;0}\} \cup \{\psi_{j;k} \ : \ n_{l,\psi} \leqslant k \leqslant 2^{j} - n_{h,\psi}\} \cup \{\psi^R_{j;2^{j}-1}\}, \quad j \geqslant J_0,$$

$\phi^R := \phi^L(1-\cdot)$, $\psi^R := \psi^L(1-\cdot)$, and $\tilde{\mathcal{B}}^{1\mathrm{D}}_{J_0}$ is similarly defined by adding $\sim$ to each element in $\mathcal{B}^{1\mathrm{D}}$.

Wavelets in Sobolev spaces

Thm Let $(\{\tilde{\phi};\tilde{\psi}\},\{\phi;\psi\})$ be any compactly supported biorthogonal wavelet in $L_2(\mathbb{R})$ such that every entry of ϕ belongs to $H^1(\mathbb{R})$. Let $(\tilde{\mathcal{B}}^{1D,x}_{J_0},\mathcal{B}^{1D,x}_{J_0})$ and $(\tilde{\mathcal{B}}^{1D,y}_{J_0},\mathcal{B}^{1D,y}_{J_0})$ be biorthogonal wavelets in $L_2(\mathcal{I})$ from $(\{\tilde{\phi};\tilde{\psi}\},\{\phi;\psi\})$ such that

$$\mathcal{B}^{1D,x}_{J_0} \subseteq \{f \in H^1(\mathcal{I}) \ : \ f(0)=f(1)=0\},$$
$$\mathcal{B}^{1D,y}_{J_0} \subseteq \{f \in H^1(\mathcal{I}) \ : \ f(0)=0\}.$$

Define $\mathcal{B}^{2D}_{J_0} := \Phi^{2D}_{J_0} \cup \cup_{j=J_0}^{\infty} \Psi^{2D}_j$ with

$$\Phi^{2D}_{J_0} := \{\Phi^x_{J_0} \otimes \Phi^y_{J_0}\} \quad \text{and} \quad \Psi^{2D}_j := \{\Phi^x_j \otimes \Psi^y_j, \Psi^x_j \otimes \Phi^y_j, \Psi^x_j \otimes \Psi^y_j\},$$

and define $\tilde{\mathcal{B}}^{2D}_{J_0}$ similarly using the dual functions. Then, $(\tilde{\mathcal{B}}^{2D}_{J_0},\mathcal{B}^{2D}_{J_0})$ is a biorthogonal wavelet basis in $L_2(\Omega)$ and

$$\mathcal{B}^{\mathcal{H}}_{J_0} := [2^{-J_0}\Phi^{2D}_{J_0}] \cup \cup_{j=J_0}^{\infty} [2^{-j}\Psi^{2D}_j]$$

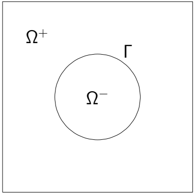
is a Riesz basis of the Sobolev space

$$\mathcal{H}(\Omega) := \{u \in H^1(\Omega) : u = 0 \text{ on } \partial\Omega \backslash \Gamma\}.$$

Elliptic interface problems

Consider the following problem

$$
\begin{aligned}
&-\nabla\cdot(a\nabla u) = f \quad \text{in} \quad \Omega\setminus\Gamma,\\
&[\![u]\!] = g, \quad [\![a\nabla u\cdot\nu]\!] = g_\Gamma \quad \text{on} \quad \Gamma,\\
&u = g_b \quad \text{on} \quad \partial\Omega,
\end{aligned}
$$



where $\Omega := (0,1)^2$, Γ is a smooth interface curve,

$$[\![v]\!](x) := \lim_{y\in\Omega_+, y\to x} v(y) - \lim_{z\in\Omega_-, z\to x} v(z) \quad \text{for} \quad x\in\Gamma,$$

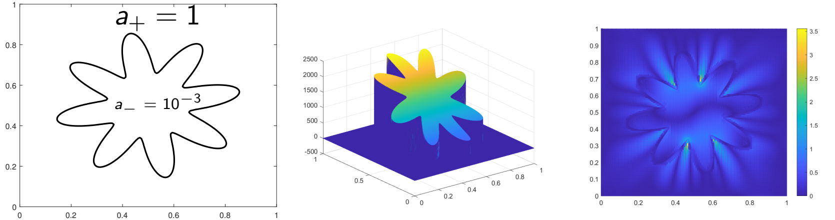
$a\in L_\infty(\Omega)$ with $\text{ess-inf}_{x,y\in\Omega}\, a(x,y) > 0$, $f\in L_2(\Omega)$, $g_\Gamma \in H^{-1/2}(\Gamma)$, and $g, g_b \in H^{1/2}(\partial\Omega)$.

Example

Let $a_+ = 1$, $a_- = 10^{-3}$, and f, g, g_Γ, g_b be chosen so that

$$u_+ = \cos(4x-2), \quad u_- = 10^3 \sin(4y-2) + 1500.$$

This makes $g, g_\Gamma \neq 0$ on Γ, and $g_b \neq 0$ on $\partial\Omega$.



J	$\mathcal{B}^{S,H_0^1(\Omega)}_{3,J}$ (ours)						$\mathcal{B}^{2D,H_0^1(\Omega)}_{3,J}$ (traditional) or Φ^{2D}_J (FEM)				
J	N_J	cond	$\frac{\|u-u_J\|_2}{\|u\|_2}$	order	$\frac{\|\nabla u-\nabla u_J\|_2}{\|\nabla u\|_2}$	order	N_J	$\frac{\|u-u_J\|_2}{\|u\|_2}$	order	$\frac{\|\nabla u-\nabla u_J\|_2}{\|\nabla u\|_2}$	order
4	4585	5.33E+3	1.27E-1		3.85E-1		225	2.47E-1		7.19E-1	
5	22857	8.23E+3	3.01E-2	1.79	1.98E-1	0.828	961	1.82E-1	0.417	5.30E-1	0.420
6	97497	9.71E+3	7.79E-3	1.86	9.27E-2	1.05	3969	9.62E-2	0.900	3.51E-1	0.580
7	398713	1.08E+4	1.58E-3	2.26	4.71E-2	0.961	16129	5.24E-2	0.866	2.44E-1	0.519

Neural networks

For a given activation function σ, the function $\phi : \mathbb{R}^{d_{\text{in}}} \to \mathbb{R}^{d_{\text{out}}}$ is a σ network with $L \in \mathbb{N}$ layers if

$$\phi := \mathcal{L}_L \circ \sigma \circ \mathcal{L}_{L-1} \circ \sigma \circ \cdots \circ \sigma \circ \mathcal{L}_1 \circ \sigma \circ \mathcal{L}_0,$$

where

- $\mathcal{L}_i(y_i) := W_i y_i + b_i$, $W_i \in \mathbb{R}^{N_{i+1} \times N_i}$, $y_i \in \mathbb{R}^{N_i}$, $y_i \in \mathbb{R}^{N_i}$,
- $N_0 = d_{\text{in}}$, $N_{L+1} = d_{\text{out}}$,
- $b_i \in \mathbb{R}^{N_{i+1}}$, and
- the activation function is applied elementwise.

Let θ denote all trainable parameters in the network. In what follows, we use ϕ_θ to emphasize the dependence on θ.

Physics-informed neural networks (PINN)

Original paper: Raissi, Perdikaris, and Karniadakis (2019).

Consider the following PDE:

$$
\begin{aligned}
&u_t + \mathcal{L}[u] = 0, \quad x \in \Omega,\ t \in [0, T],\\
&u(x,0) = g(x), \quad x \in \partial\Omega,\\
&\mathcal{B}[u] = 0, \quad x \in \partial\Omega,\ t \in [0, T],
\end{aligned}
$$

where

- $\mathcal{L}[\cdot]$ is a linear or nonlinear differential operator, and
- $\mathcal{B}[\cdot]$ is a boundary operator such as Dirichlet, Neumann, Robin, or periodic boundary conditions.

Physics-informed neural networks (PINN)

Define the PDE residuals as

$$\mathcal{R}_\theta(x,t) := \frac{\partial \phi_\theta(x,t)}{\partial t} + \mathcal{L}[\phi_\theta](x,t).$$

Suppose that $\{x_{\mathrm{ic}}^i\}_{i=1}^{N_{\mathrm{ic}}} \subset \partial\Omega$, $\{x_{\mathrm{bc}}^i, t_{\mathrm{bc}}^i\}_{i=1}^{N_{\mathrm{bc}}} \subset \partial\Omega \times [0,T]$, and $\{x_{\mathrm{r}}^i, t_{\mathrm{r}}^i\}_{i=1}^{N_{\mathrm{r}}} \subset \Omega \times [0,T]$.

Then, we minimize the following sum of loss functions

$$\mathcal{L}(\theta) = \mathcal{L}_{\mathrm{ic}}(\theta) + \mathcal{L}_{\mathrm{bc}}(\theta) + \mathcal{L}_{\mathrm{r}}(\theta),$$

where

$$\mathcal{L}_{\mathrm{ic}}(\theta) = \frac{1}{N_{\mathrm{ic}}} \sum_{i=1}^{N_{\mathrm{ic}}} |\phi_\theta(x_{\mathrm{ic}}^i, 0) - g(x_{\mathrm{ic}}^i)|^2, \quad \mathcal{L}_{\mathrm{bc}}(\theta) = \frac{1}{N_{\mathrm{bc}}} \sum_{i=1}^{N_{\mathrm{bc}}} |\mathcal{B}[\phi_\theta](x_{\mathrm{bc}}^i, t_{\mathrm{bc}}^i)|^2,$$

$$\mathcal{L}_{\mathrm{r}}(\theta) = \frac{1}{N_{\mathrm{r}}} \sum_{i=1}^{N_{\mathrm{r}}} |\mathcal{R}_\theta(x_{\mathrm{r}}^i, t_{\mathrm{r}}^i)|^2.$$

Let's do a demo.

Neural operators: DeepONet

Original paper: Lu, Jin, Pang, Zhang, and Karniadakis (2021).

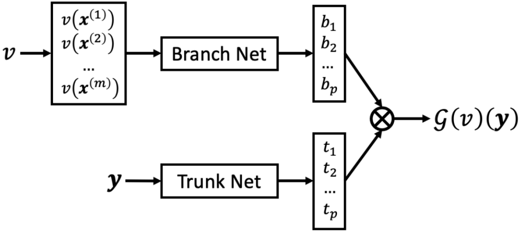
DeepONet aims to approximate an operator (the mapping from functions to functions). Define the target nonlinear operator as

$$\mathcal{G} : v \mapsto u,$$

where

$$v : x \mapsto v(x) \in \mathbb{R},\ x \in D \subset \mathbb{R}^d, \quad \text{and} \quad u : y \mapsto u(y) \in \mathbb{R},\ y \in D' \subset \mathbb{R}^{d'}.$$

The vanilla DeepONet has two parts: branch and trunk networks.



Neural operators: DeepONet

Consider the following PDE

$$\mathcal{L}[u; k] = f, \quad x \in \Omega,$$
$$\mathcal{B}[u] = g, \quad x \in \partial\Omega,$$

where $\mathcal{L}$ is a differential operator, $\mathcal{B}$ is the boundary operator, and $k = k(x)$ parameterizes $\mathcal{L}$.

Goal: use DeepONet to approximate the solution operator $\mathcal{G} : k, f \mapsto u$.

How to train?

- Generate many $(\tilde{k}, \tilde{f})$ pairs, say M pairs.
- For each pair, use classical discretization method to obtain an approximated solution, $\tilde{u}$.
- Train the DeepONet by using $\{(\tilde{k}_i, \tilde{f}_i)\}_{i=1}^{M}$ as inputs and $\{\tilde{u}_i\}_{i=1}^{M}$ as the output.

Let's do a demo.