Fast Physics Informed Kernel Methods for Nonlinear PDEs with Unknown Coefficients

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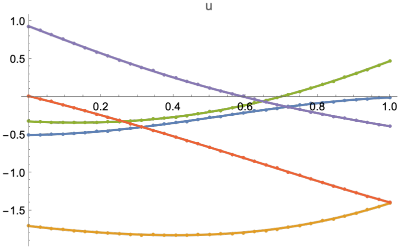
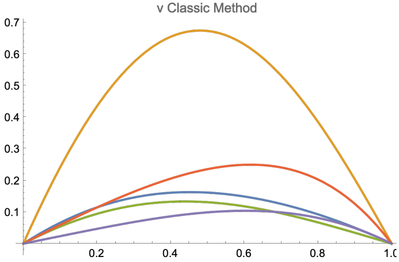
Solving PDEs with Machine Learning

Example PDE: $e^{u(x)}\left[u_x(x)v_x(x) + v_{xx}(x)\right] = -1, \qquad v(0) = 0 = v(1)$

- Try to approximate solution v when input u either deterministic or random
- ML approaches to approximate $u \mapsto v$ include neural networks and kernel methods
- PDE may be non-linear and high dimensional
- Physics informed ML does not rely on reference solver data e.g. finite difference





Neural Networks and Kernel Methods for Solving PDEs

	PDE with deterministic coefficients		PDE with unknown coefficients	
	reference solver	physics informed	reference solver	physics informed
neural networks	[Abiodun et al., 2018]	[Raissi et al., 2019]	[Lu et al., 2021]	[Wang et al., 2021]
kernel methods	[Williams and Rasmussen, 2006]	[Chen et al., 2021]	[Batlle et al., 2024]	proposed solution

- Physics Informed Neural Networks (PINN) [Raissi et al., 2019]
  Loss function of PDE equations using automatic differentiation
- Deep Operator Networks (DeepONets) [Lu et al., 2021]
  Combine network for x with network for u [Wang et al., 2021]

	scalability	convergence guarantees	error rates	interpretability
neural networks	$+$	$+$	$\pm$	$-$
kernel methods	$\pm$	$+$	$+$	$+$

Operator Learning Framework

$$e^{u(x)}\left[u_x(x)v_x(x) + v_{xx}(x)\right] = -1, \qquad v(0) = 0 = v(1)$$

- $u \in \mathcal{U}$ has known distribution and u_x available e.g. a Gaussian process
- $v \in \mathcal{V}$ to be solved for
- **Goal:** Find operator $G^\dagger(u) = v$
- $\phi(u) = (\phi_1(u), \ldots, \phi_n(u))$ linear samples of u e.g. $\phi(u) = (u(x_1), u(x_2), \ldots, u_x(x_1), u_x(x_2), \ldots)$
- $\varphi(v) = (\varphi_1(v), \ldots, \varphi_m(u))$ linear sampler of v e.g. $\varphi(u) = (v(0), v(1), v_x(x_1), v_x(x_2), \ldots, v_{xx}(x_1), v_{xx}(x_2), \ldots)$

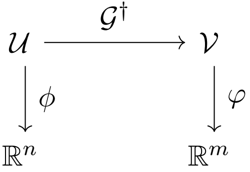
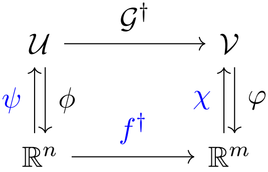


Diagram and framework of [Batlle et al., 2024]

Operator Learning Framework Continued

$$e^{u(x)}\left[u_x(x)v_x(x) + v_{xx}(x)\right] = -1, \qquad v(0) = 0 = v(1)$$

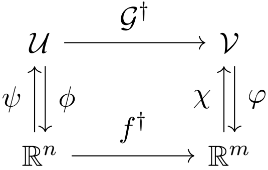
- $\psi(\phi(u)) = \hat{u}$ approximates u from samples $\phi(u) \in \mathbb{R}^n$
- $\chi(\varphi(v)) = \hat{v}$ approximations v from samples $\chi(v) \in \mathbb{R}^m$
- $f^\dagger(\phi(u)) \approx \varphi(v)$ approximates samples of v from samples of u
- $G^\dagger \approx \chi \circ f^\dagger \circ \phi$
  1. Samples u to get $\phi(u)$
  2. Approximates v samples $\varphi(v)$ by $f^\dagger(\phi(u))$
  3. Reconstructs approximate v as $\chi(f^\dagger(\phi(u)))$ from samples

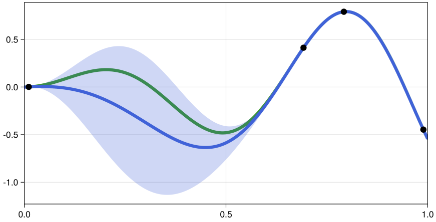


Kernel Methods Idea

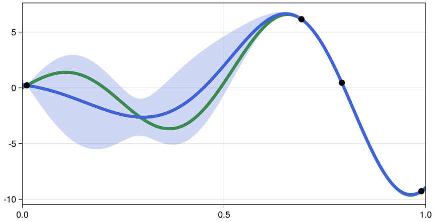
Use RKHS kernel interpolant for ψ, χ, and $f^\dagger$

- ψ rarely used to reconstruct input u
- $f^\dagger$ a vector valued kernel interpolant
- χ an optimal reconstruction map in RKHS
- May reinterpret kernel interpolants as Gaussian processes





GP



GP derivative

Physics Informed Kernel Methods

1. Pick a realization $u \in \mathcal{U}$
2. Sample $\phi(u) \in \mathbb{R}^n$
3. Optimize unknown $\varphi(v) \in \mathbb{R}^m$ to minimize RKHS interpolant norm satisfying PDE
4. Repeat 1. to 3. for many realizations of $u_1, \ldots, u_N$
5. Build kernel interpolant $f^\dagger$ from $\{\phi(u_i)\}_{i=1}^N$ and optimized $\{\varphi(v_i)\}_{i=1}^N$
6. Use mapping $f^\dagger$ and optimal recovery map χ on unseen $\phi(u^*)$

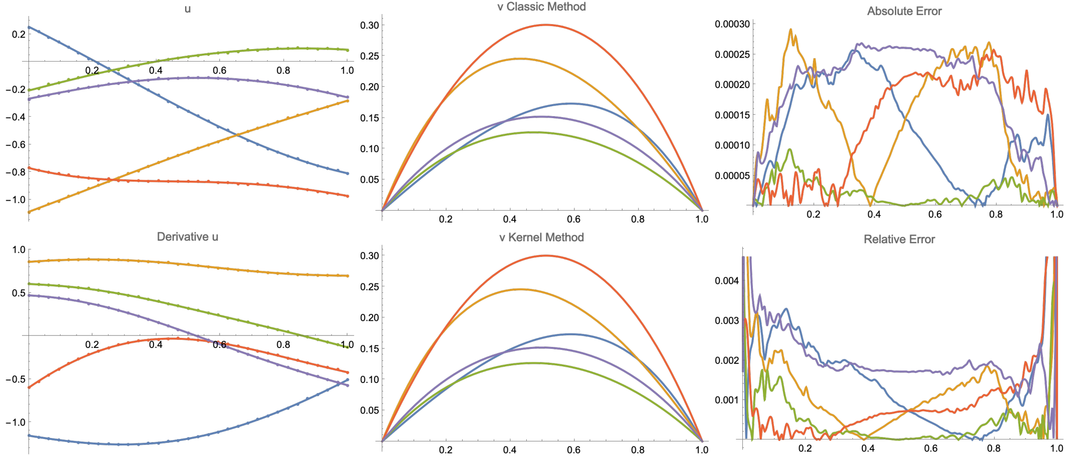
Connections to Existing Kernel Methods for PDEs

- [Chen et al., 2021] is 1. to 3. for deterministic u
- [Batlle et al., 2024] is 5. and 6. for unknown u when reference solver available

Idea: Use physics informed kernel method for deterministic u as the reference solver in kernel operator learning framework

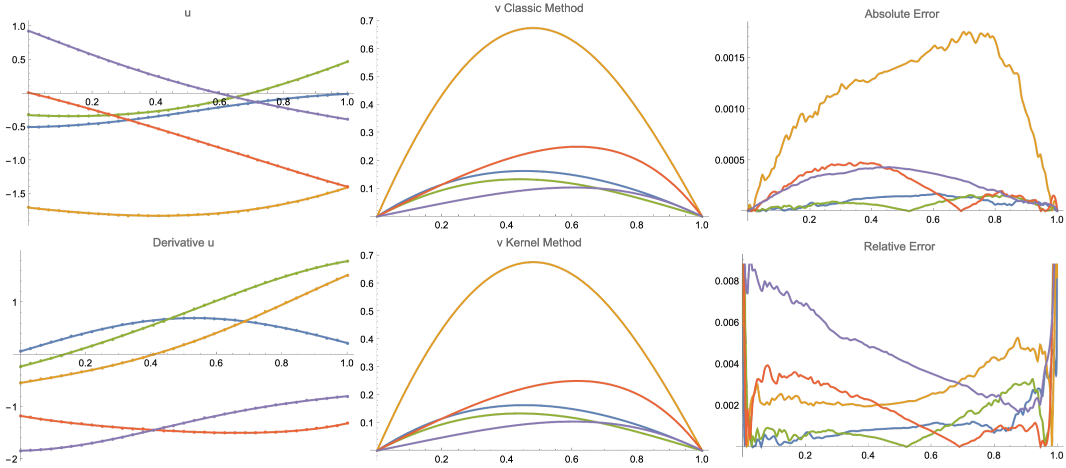
Train 1D Elliptic PDE

$$e^{u(x)}\left[u_x(x)v_x(x)+v_{xx}(x)\right]=-1,\quad v(0)=0=v(1)$$



Test 1D Elliptic PDE

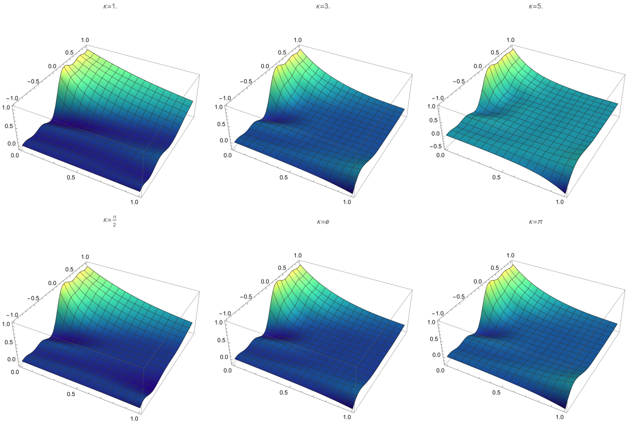
$$e^{u(x)}\left[u_x(x)v_x(x)+v_{xx}(x)\right]=-1,\quad v(0)=0=v(1)$$



Radiative Transfer Equation 1D

Top Row Train. Bottom Row Test

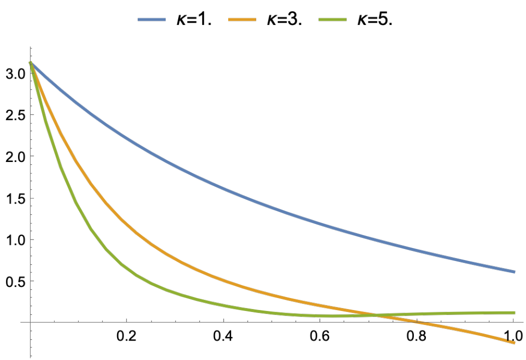
$$sv_x(x,s)+kv(x,s)=0, \qquad v(0,s>0)=1, \qquad v(1,s<0)=0, \qquad \text{scalar } k \text{ unknown}$$

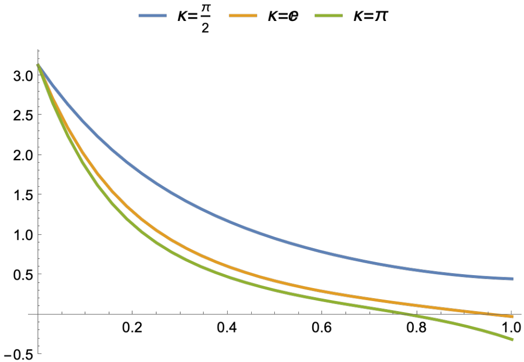


Heat Flux from Radiative Transfer Equation 1D

Left Train. Right Test

$$s v_x(x,s) + \kappa v(x,s) = 0, \qquad v(0, s>0) = 1, \qquad v(1, s<0) = 0,$$ scalar k unknown





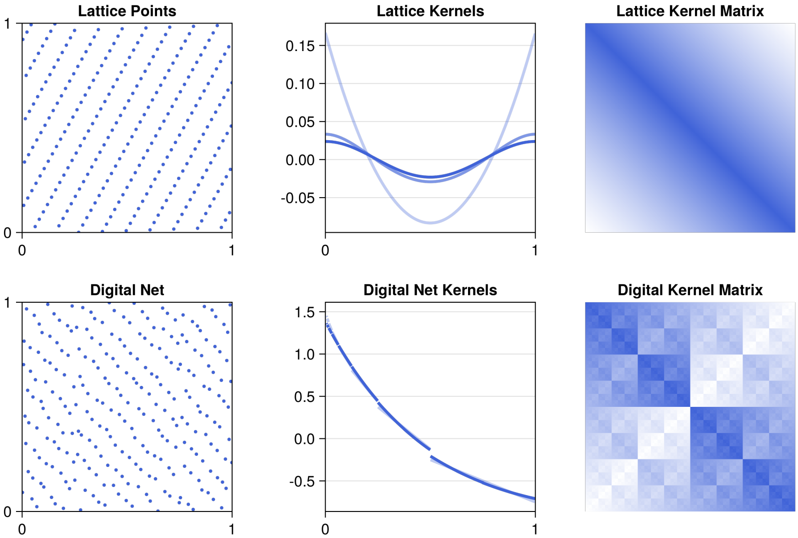
Fast Kernel Methods via Structured Gram Matrices

- RKHS kernel $\mathcal{K} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ yields Gram matrix $\mathsf{K} = (\mathcal{K}(x_i, x_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}$
- Kernel interpolant fit by solving linear system $\mathsf{K}a = b$ for a
- Choose $\mathcal{K}$ and $\{x_i\}_{i=1}^n$ to induce structure in K allowing faster solve $\mathsf{K}a = b$

samples $\{x_i\}_{i=1}^n$	kernel $\mathcal{K}$	Gram matrix K	Solving $\mathsf{K}a = b$
unstructured	general	dense unstructured	$\mathcal{O}(n^3)$
regular grid	stationary	block Circulant	$\mathcal{O}((n \log n)^d)$
lattice sequence	shift-invariant	circulant	$\mathcal{O}(n \log n)$
digital sequence	digitally shift invariant	block Toeplitz	$\mathcal{O}(n \log n)$

My PhD research extends fast kernel methods with lattice and digital sequence [Jagadeeswaran and Hickernell, 2019, 2022] to accommodate derivative information

Fast Quasi-Monte Carlo Kernel Interpolation



Discussion

Observations

- Proposed method simply couples existing kernel methods for
  1. Solving PDEs with deterministic coefficients [Chen et al., 2021]
  2. Operator learning when a reference solver is available [Batlle et al., 2024]
- Mathematica supports symbolic linear functionals e.g. derivatives and integrals
  - Symbolic computations can sometimes be prohibitively slow
  - Potential opportunity to expand kernel methods to weak formulations

Future Work

- Derive convergence guarantees and rates
- Implement fast kernel methods for this setting
- Apply to challenging PDEs in high dimensions

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