Learning solution operators for PDEs with uncertainty

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How do we solve a PDE?

Operator learning problem

Let $\mathcal{L}_\lambda$ be a differential operator depending on a parameter $\lambda \in \mathcal{A}$.

We want to find the solution $u(x)$ of the PDE

$$\begin{aligned} &\left(\mathcal{L}_\lambda u\right)(x) = f(x) && x \in D \subset \mathbb{R}^d \\ &\text{boundary condition} && x \in \partial D \end{aligned} \tag{1}$$

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Equation (1) defines a solution operator

$$\mathcal{H} : \Lambda \times \mathcal{F} \longrightarrow \mathcal{U}$$
$$(\lambda, f) \longmapsto u_{\lambda,f} \quad \text{solution of (1)}$$

Case 1. λ *fixed*, f varies. $\rightarrow \quad \mathcal{G}: \ f \mapsto u$

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If the differential operator $\mathcal{L}_\lambda$ is *linear*, and a Green's function $G : DxD \rightarrow \mathbb{R}$ exists for the operator $\mathcal{L}_\lambda$, we can express the solution $u(x)$ of $\left(\mathcal{L}_\lambda u\right)(x) = f(x)$ as

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We consider the operator

$$\mathcal{G}: \mathcal{F} \longrightarrow \mathcal{U}$$

$$f \longmapsto u(x) = \int_D G_\lambda(x,y)\, f(y)\, dy$$

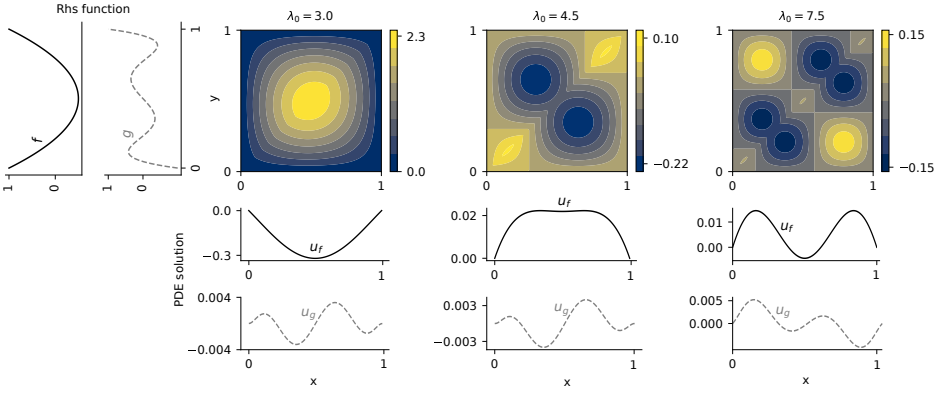
Note that $\mathcal{G} = \mathcal{L}_\lambda^{-1}$ Inverse problem

Linear PDEs and Green's function

A visualization

Example: $(\mathcal{L}_\lambda u)(x) = -\left(\frac{d}{dx^2} + \lambda\right) u(x) = f(x) \quad x \in [0,1], \quad u(0) = u(1) = 0$

with Green's function $G_\lambda(x,y) = \frac{1}{\lambda \sin \lambda}\left[\Theta(y-x)\sin(\lambda x)\sin(\lambda(1-y)) + \Theta(x-y)\sin(\lambda(1-x))\sin(\lambda y)\right]$



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i.e. inferring the Green's function

Solution operator ($\lambda \in \mathbb{R}$ fixed)

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We want to learn $\mathcal{G}$ in a probabilistic framework.

Gaussian Process regression

with Integral observations

Define the integral operator $\mathcal{A}_f = \mathcal{A}$ acting on G as $\mathcal{A}G = \int_D G(\cdot, y)f(y)dy = u(\cdot)$.

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Posterior mean and covariance

$$\mathbb{E}[G] = \mu + \mathcal{A}^* k_\theta (\mathcal{A}\mathcal{A}^* k_\theta + \sigma^2)^{-1}(u - \mathcal{A}\mu)$$

$$\mathrm{Cov}(G) = k_\theta - \mathcal{A}^* k_\theta (\mathcal{A}\mathcal{A}^* k_\theta + \sigma^2)^{-1}\mathcal{A}k_\theta.$$

where

$$\mathcal{A}^* k_\theta = \int_D k_\theta((x, y), (X, \tau))f(\tau)d\tau, \quad \mathcal{A}\mathcal{A}^* k_\theta = \int_D k_\theta((X, \tau_1), (X, \tau_2))f(\tau_1)f(\tau_2)d\tau_1 d\tau_2$$

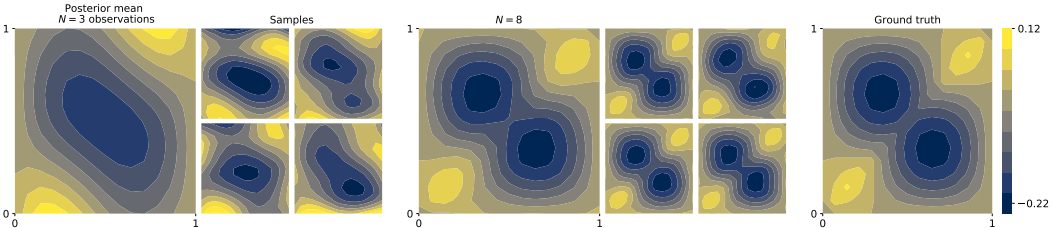
(when discretized $\mathcal{A}\mathcal{A}^* k_\theta = A k_\theta A^T$)

An experiment

Posterior distribution on the operator

$$(\mathcal{L}_\lambda u)(x) = (-\Delta - \lambda^2) u(x) = f(x) \quad x \in [0,1], \quad \lambda = 4.5 \quad u(0) = u(1) = 0$$

Data $\{f_i, u_i\}_{i=1}^N$, Product kernel $k((x,x'),(y,y')) = k_1(x,y)\, k_2(x',y')$



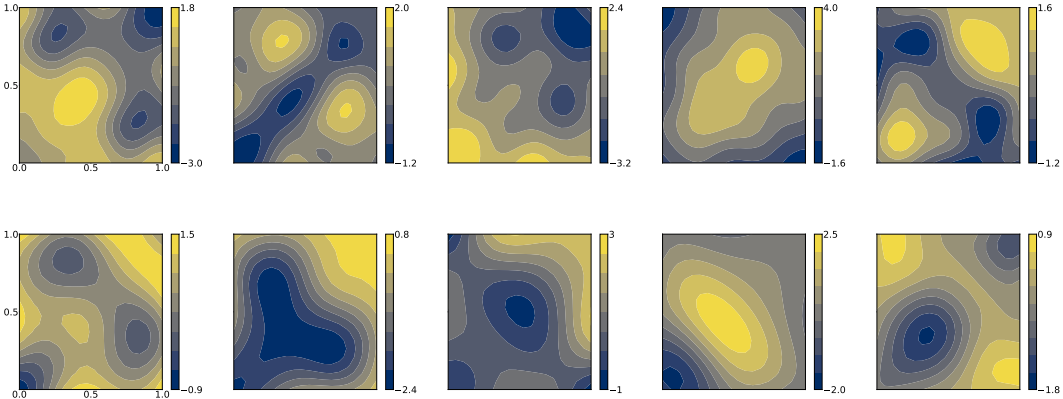
Posterior on G and ground truth [Magnani et al. 2022]

Encoding symmetries in the kernel

Prior knowledge

We can encode prior knowledge about the Green's function in the choice of our kernel.

For the Green's function $G(x_1, x_2) = G(x_2, x_1)$.



Deep neural networks to solve PDEs

Neural operators, FNO ... [Lu et al 2021] [Li et al 2020,2021] [Kowachki et al 2021]

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through the composition of L layers $(\lambda, f) \longmapsto (\psi_L \circ \cdots \circ \psi_1)(\lambda, f)$

An iterative solver $\underbrace{\psi_{i+1}(f,\lambda) = \sigma\left(W_i\psi_i(x) + \int_D \overbrace{g_\theta(x,y,\lambda)}^{\text{NN1}}\, \psi_i(y)\, dy\right)}_{\text{NN2}}$ $\qquad i = 0, \dots N$

$\rightarrow$ **Case 1** gives a theoretical understanding to these complex architectures

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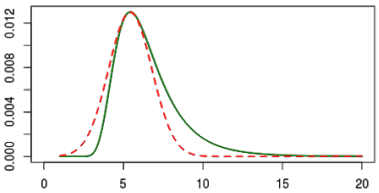
Uncertainty becomes even more important

Uncertainty with Laplace approximation (LA)

Old but gold



$q(\theta) = \log h(\theta)$ Taylor expansion of $q(\theta)$ around the mode $\hat{\theta}$:

$$q(\theta) \approx q(\hat{\theta}) + \overbrace{q'(\hat{\theta})(\theta - \hat{\theta})}^{=0} + \frac{1}{2}(\theta - \hat{\theta})q''(\hat{\theta})(\theta - \hat{\theta})$$

$$= c - \frac{(\theta - \mu)^2}{2\sigma^2} \rightarrow \log \mathcal{N}(\mu, \sigma^2), \quad \mu = \hat{\theta}, \quad \sigma^2 = (-q(\hat{\theta})'')^{-1}$$

Laplace approximation in Deep learning

[MacKay 1992], [Daxberger, Kristiadi, Immer, Eschenhagen, Bauer, Hennig 2021]

Consider a deep network $f_\theta : \mathbb{R}^m \to \mathbb{R}^n$ trained on $\mathcal{D} = (x_i \in \mathbb{R}^m, y_i \in \mathbb{R}^n)_{i=1}^N$ to find

$$\theta_{\text{MAP}} = \arg\min_\theta \mathcal{L}(\mathcal{D};\theta) = \arg\min_\theta \left(\frac{1}{N} \sum_1^N L(x_n, y_n; \theta) + r(\theta) \right)$$

$$= \arg\max_\theta - \Big(\log p(y|f_\theta(x)) + \log p(\theta) \Big) = \arg\max_\theta p(\theta|y)$$

$$\boxed{p(\theta|\mathcal{D}) \approx \mathcal{N}(\theta_{\text{MAP}}, \Sigma) \quad \text{with } \Sigma = -(\nabla^2_\theta \mathcal{L}(\mathcal{D};\theta))^{-1}}$$

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..and a gaussian distribution over the (linearized) network output

$$p(f(x) \mid x, D) \approx \mathcal{GP}\big(f;\ f_{\theta_{\text{MAP}}}(x),\ J(x)^T \Sigma J(x)\big) \quad \text{with } J = \nabla_\theta f_\theta(x)|_{\theta_{\text{MAP}}}$$

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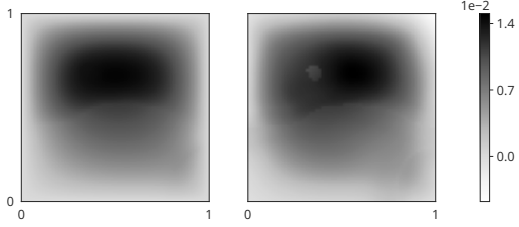
$\to$ Small computational overhead!

Uncertainty estimates on a Darcy flow

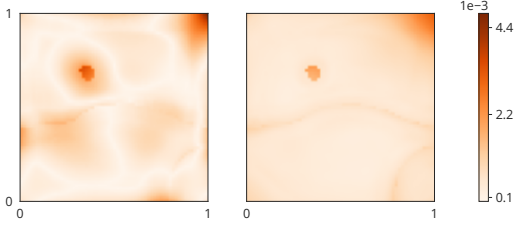
[Li, Kovachki, Azizzadenesheli, Liu, Bhattacharya, Stuart, Anandkumar, 2020]

Darcy flow in $D = [0,1]^2$

$$-\nabla \cdot (\lambda(x)\nabla u(x)) = f(x), \quad x \in D$$
$$u(x) = 0 \qquad x \in \partial D$$



Ground truth and approximation



Error and standard deviation [Magnani et al. 2022]

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Low-data regime

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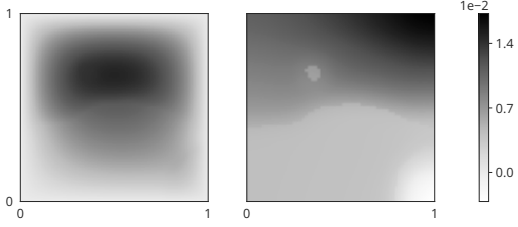

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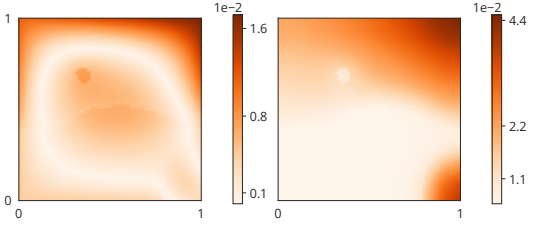

Error and standard deviation

Operator learning in the context of inverse problems

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$\rightarrow$ inverse problem

$$u = \mathcal{A}_f g + \varepsilon \qquad \text{with} \qquad \mathcal{A}_f g = \int g(x,y)f(y)\,dy$$

Classical inverse problem setting $u = \mathcal{A}g + \varepsilon$ $\mathcal{A}$ given, $(g_i, u_i)_{i=1}^N$

$\longrightarrow$ learn $\hat{F} =$ "$\mathcal{A}^{-1}$" *stable* such that for a new u_*, $g_* \approx \hat{F}(u_*)$

Convolution operators

A special case, a starting point

Integral operator, for $\mathcal{F}, \mathcal{U}$ Hilbert spaces $\mathcal{G} : \mathcal{F} \to \mathcal{U}$ $\quad f \mapsto u(x) = \int G(x,y) f(y)\, dy$.

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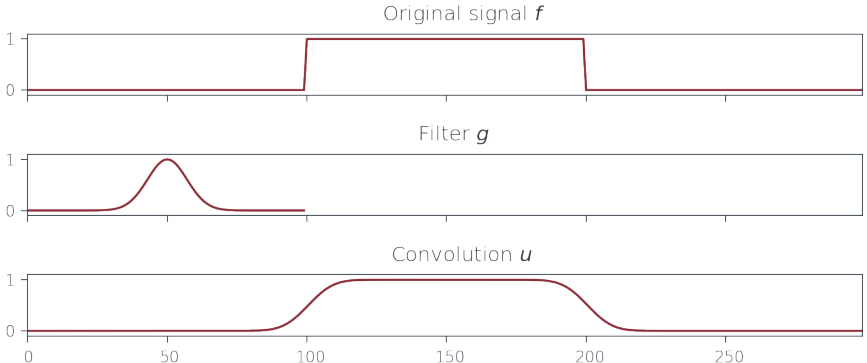

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- Special family of of PDEs
- Learning an operator with structure: known diagonalization! (Fourier basis)
- Convolution are at the core of many applications

Let L be a differential operator

$$L = \sum_{\alpha \leq m} C_\alpha D^\alpha$$

A function $U \in \mathcal{D}(\mathbb{R}^n)$ that satisfies

$$LU = \delta$$

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Important examples for L are

Laplacian $\Delta_x = \sum_i \frac{\partial^2}{\partial x_i^2}$ Heat operator $\partial_t - \Delta_x$ Wave operator $\partial_{tt} - c^2 \Delta_x$

1d Heat equation

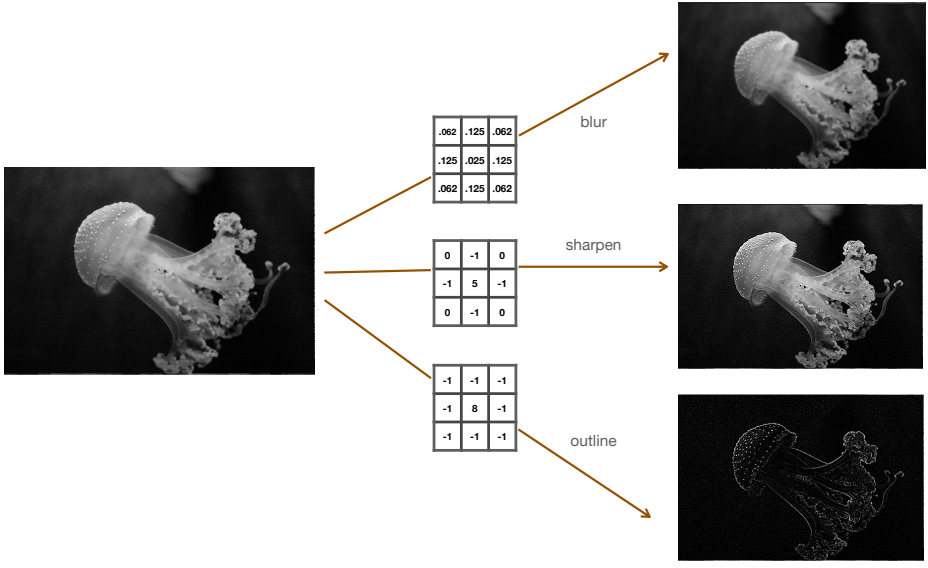
$$\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}u(x,t) \tag{3}$$

Numerical algorithms for solving PDEs (e.g. method of lines) discretize in space on a mesh $D = \{x_1, x_1 + h ... x_1 + dh\}$ and solve in time.
So (3) becomes

$$\frac{\partial}{\partial t}u_d = \frac{K}{h^2}u_d \quad \text{with} \quad K = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{bmatrix} \quad \text{and} \quad h = \frac{1}{d+1}$$

Second derivative is replaced by second differences at grid points:

$$\frac{\partial^2}{\partial x^2}u(x,t) = \frac{u(x-h,t) - 2u(x,t) + u(x+h,t)}{h^2}$$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-1 8 -1
-1 -1 -1
outline

4. Probability theory

See: 3blue1Brown for a better visualization

The probability distribution of the sum of two independent random variables is the convolution of their individual distributions.

$$Z = X + Y, \quad P(Z = z) = \sum_{k} P(X = k)P(Y = z - k)$$

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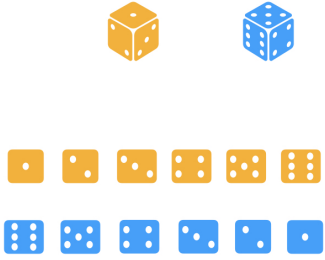

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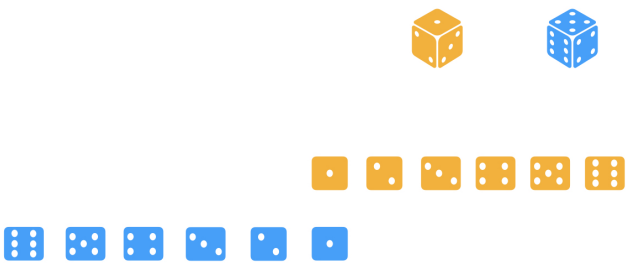

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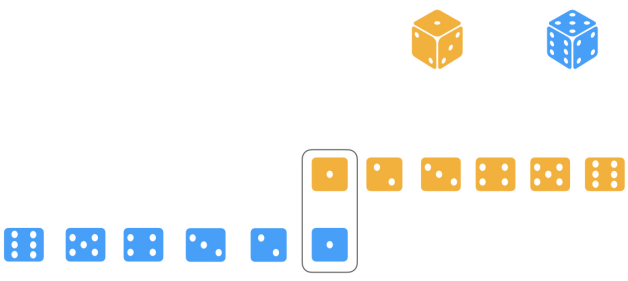

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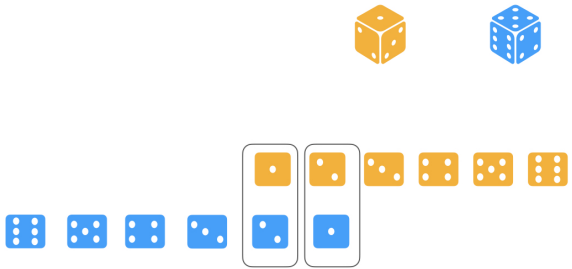

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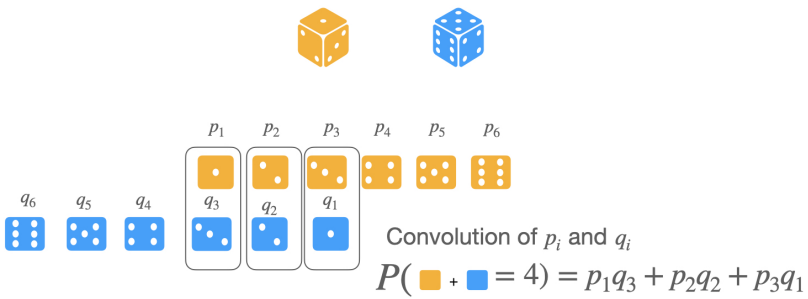

So many convolutions!

Operation that shows up in a lot of seemingly unrelated areas.

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Kernel ridge regression. $\mathcal{H}$ RKHS

$$\tilde{w} = \arg\min_{w \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left\| F_w(x_i) - y_i \right\|_{\mathcal{Y}}^2 + \lambda \left\| w \right\|_{\mathcal{H}}^2$$

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For convolution operators

1. Transposition of the problem: operator valued kernels become tractable
2. Interpretable source conditions

Operator valued kernels

An overview

Scalar case $y_i = f(x_i) + \varepsilon_i, \quad f\colon \mathcal{X} \to \mathcal{Y}, \quad \mathcal{X} = \mathbb{R}^d, \quad \mathcal{Y} = \mathbb{R}$

- $\mathcal{H}$ parameter (Hilbert) space
- Feature map $\phi\colon \mathcal{X} \to \mathcal{H}$, search for $f_w(x) = \langle w, \phi(x) \rangle_{\mathcal{H}} \in \mathcal{Y}, \quad w \in \mathcal{H}$
- $\mathcal{F} = \{f_w | w \in \mathcal{H}\}$ RKHS with kernel $K\colon \mathcal{X} \times \mathcal{X} \longrightarrow \mathcal{Y}$, $K(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$

[1] See Houman Owhadi

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Vector-valued case [1] $y_i = F(x_i) + \varepsilon_i, \quad F\colon \mathcal{X} \to \mathcal{Y}, \quad \mathcal{X}, \mathcal{Y}$ separable Hilbert spaces

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Note that $\|f\|_{\mathcal{F}} = \|w\|_{\mathcal{H}}$

[1] See Houman Owhadi

Operator valued kernels for convolution

Vectorial case for convolution $y_i = \overbrace{F(x_i)}^{x_i * w} + \varepsilon_i, \quad F\colon \mathcal{X} \to \mathcal{Y}, \quad \mathcal{X} = L^1, \quad \mathcal{Y} = L^2$

- $\mathcal{H}$ (scalar) RKHS with $K(t,s) = K_0(t-s), \quad K \in L^1$
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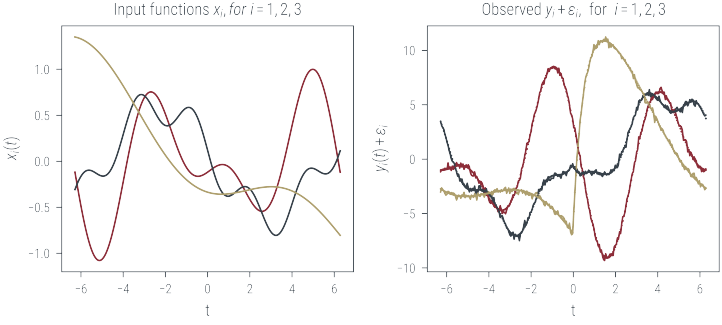
Parametrizing in frequency domain makes computation easier!

- $\Phi\colon \mathcal{X} \to \mathcal{L}(\widehat{\mathcal{H}}, \mathcal{Y})$, with $\Phi(x)w = x * \mathcal{F}^{-1}\widehat{w}$
- $\mathcal{F}\mathcal{K}(x,x')\mathcal{F}^{-1}\colon l^2 \longrightarrow l^2$ is Fourier multiplier with $\left(\mathcal{F}\mathcal{K}(x,x')\mathcal{F}^{-1}\right)_{l\,l'} = \delta_{l\,l'}\widehat{x}\widehat{K_0}\widehat{x'}$

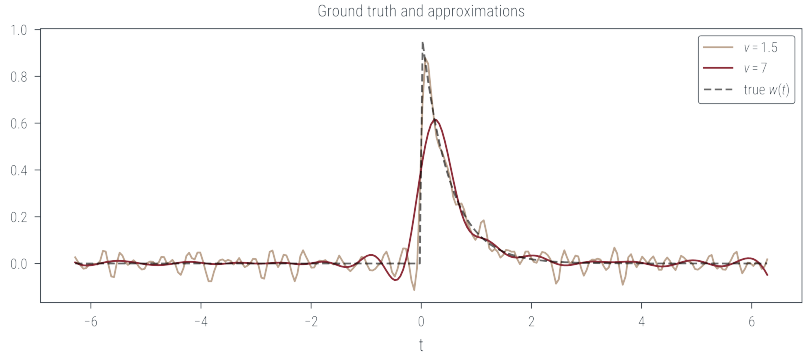
$$(\tilde{w})_l = [\ldots] = \frac{\frac{1}{n}\sum_{i=1}^n (\widehat{x}_i)_l (\widehat{y}_i)_l}{\frac{1}{n}\sum_{i=1}^n |(\widehat{x}_i)_l|^2 + \lambda \widehat{k}_l^{-1}}.$$

An example


Input functions x_i, for $i = 1, 2, 3$
$x_i(t)$
1.0
0.5
0.0
−0.5
−1.0
−6
−4
−2
0
2
4
6
t
Observed $y_i + \varepsilon_i$, for $i = 1, 2, 3$
$y_i(t) + \varepsilon_i$
10
5
0
−5
−10
−6
−4
−2
0
2
4
6
t

Changing kernel

i.e. changing RKHS/ GP covariance matrix



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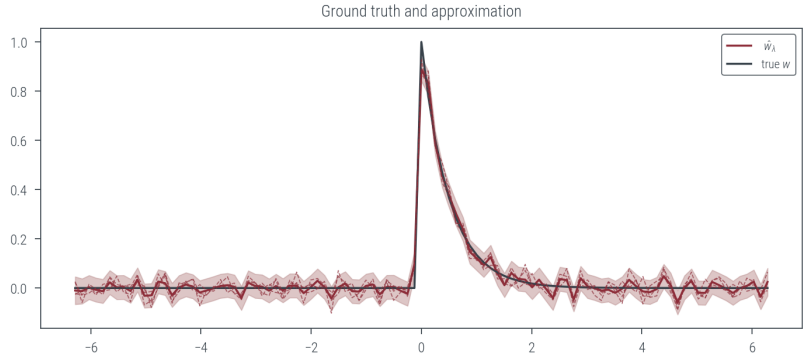

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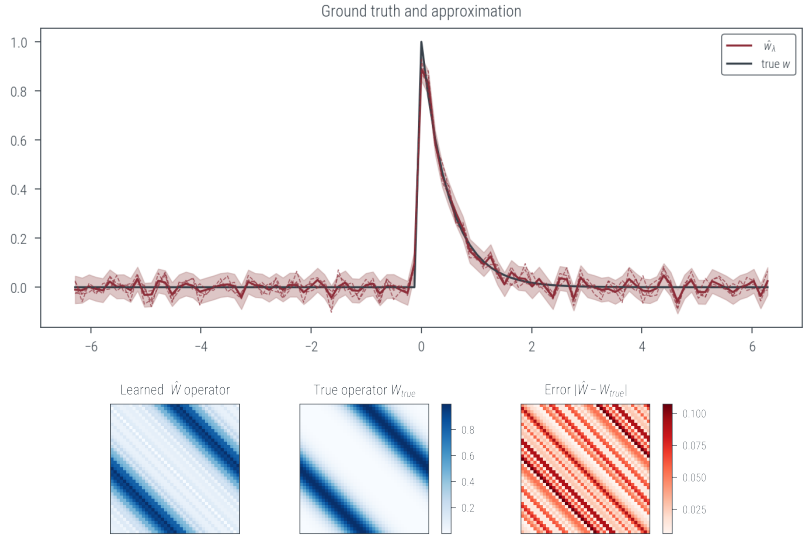

Source conditions for convolution

Convergence rates usually rely on source conditions. In general, it is difficult to formulate source conditions that are verifiable. This is not the case for convolution.

Theorem Assume $w^* \in L^2(G)$, let $(x_i, y_i)_{i=1}^N \overset{i.i.d}{\sim} \rho$ probability distribution on $\mathcal{X} \times \mathcal{Y}$,

$$\sum_{l \in \mathbb{Z}} \frac{|\widehat{w}_l^*|}{(\widehat{k}_l \mathbb{E}[|\widehat{X}_l|^2])^\alpha} < +\infty$$

and let

$$\tilde{w} = \arg\min_{w \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \|x_i * w - y_i\|_{\mathcal{Y}}^2 + \lambda_n \|w\|_{\mathcal{H}}^2$$

with regularization parameter $\lambda_n = n^{-\frac{1}{\alpha+2}}$. Then with probability at least $1 - 4e^{\tau}$

$$\|\tilde{w} - w^*\|_{L^2} \leq C\tau n^{-\frac{\alpha}{\alpha+2}}$$

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the 'fil rouge'

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- GPs for inferring the Geen's function (inverse problems)
- Generalization to deep nets: Laplace approximation
- Operator learning from data: convolution operators

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Thank you!