Machine Learning for Many-Body Systems in Physics PART 2 !

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University Kiel, 2022

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The Bottleneck

How to compute Multivariate Function Expansions that closely approximate the ground truth function ?

- **Geometric approximation rates of Fourier expansions for analytic periodic functions, FFTs**

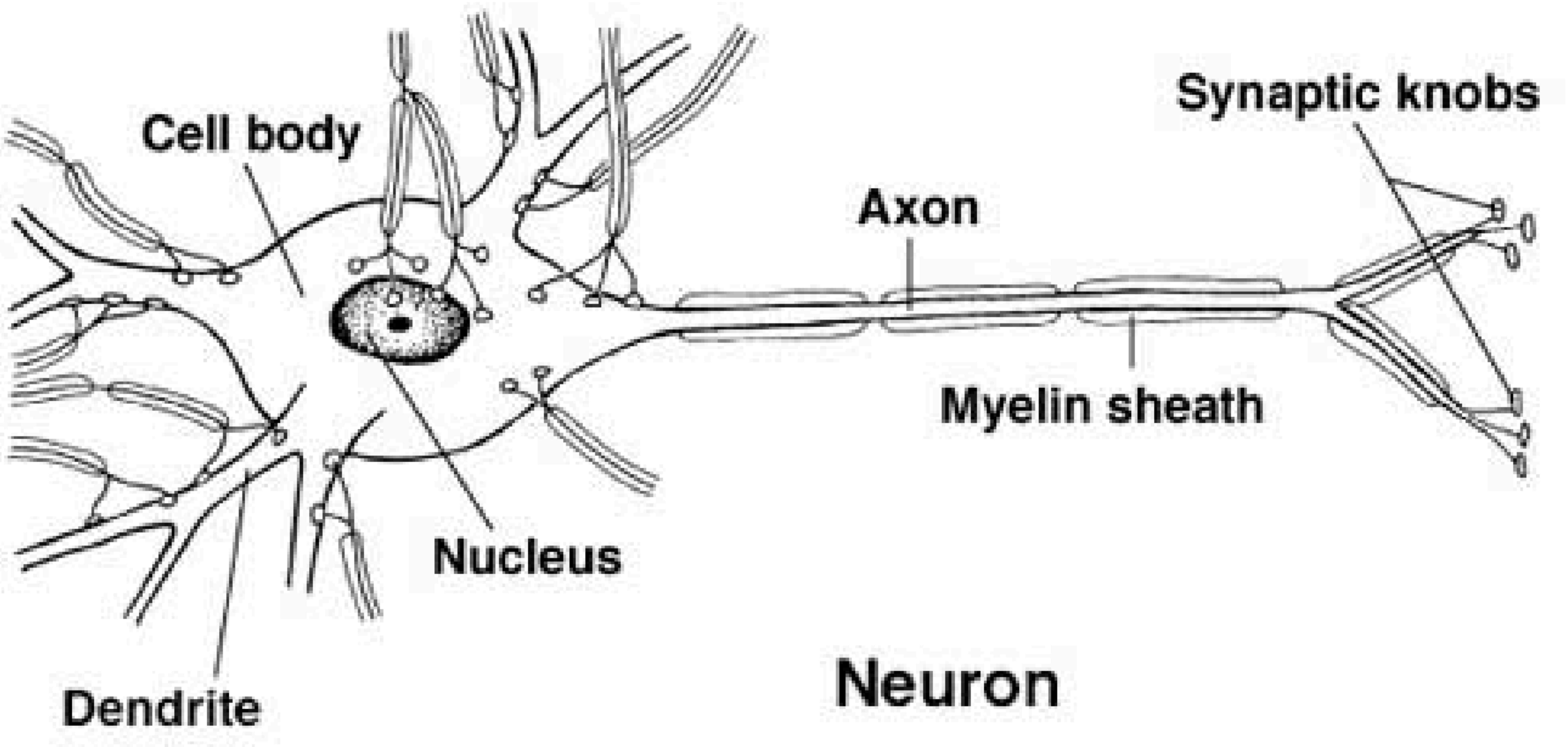
$$\theta(z) \approx \theta_n = \sum_{\|\alpha\|_\infty \leq n} c_\alpha e^{2\pi i \alpha \cdot z}, \qquad \|\theta - \theta_n\|_{C^0(\Omega)} = \mathcal{O}(r^{-n}), \qquad r > 1$$

- **Geometric approximation rates of the Coulomb / Gravitation field expansion in FMMs**

$$\phi(z) \approx \phi_n = Q \log(z) + \sum_{k=1}^{n} \frac{a_k}{z_k}, \qquad \|\phi - \phi_n\|_{C^0(\Omega)} = \mathcal{O}(z^{-n}), \qquad |z| > 1\,.$$

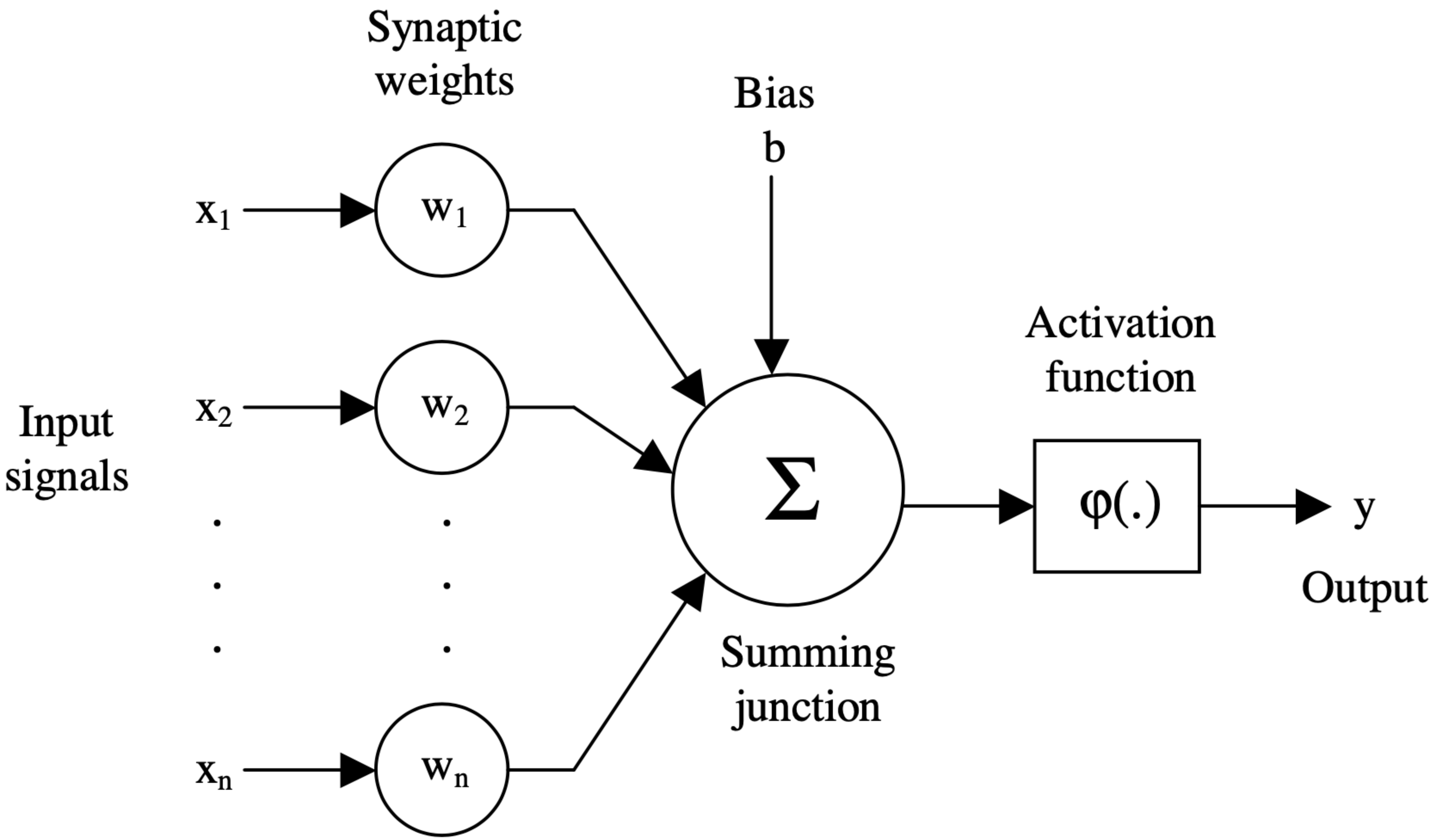
Gauss, C. F. (1886). Theoria interpolationis methodo nova tractata Werke band 3, 265–327. *Göttingen: Königliche Gesellschaft der Wissenschaften*.
Cooley, J. W., & Tukey, J. W. (1965). An algorithm for the machine calculation of complex Fourier series. *Mathematics of computation*, *19*(90), 297-301.
Greengard, L., & Rokhlin, V. (1987). A fast algorithm for particle simulations. *Journal of computational physics*, *73*(2), 325-348.

What are Neural Nets (NNs) ?



Csáji, B. C. (2001). Approximation with artificial neural networks. *Faculty of Sciences, Etvs Lornd University, Hungary*, *24*(48), 7.
Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep learning*. MIT press.

What are Neural Nets (NNs) ?



Csáji, B. C. (2001). Approximation with artificial neural networks. *Faculty of Sciences, Etvs Lornd University, Hungary*, *24*(48), 7.
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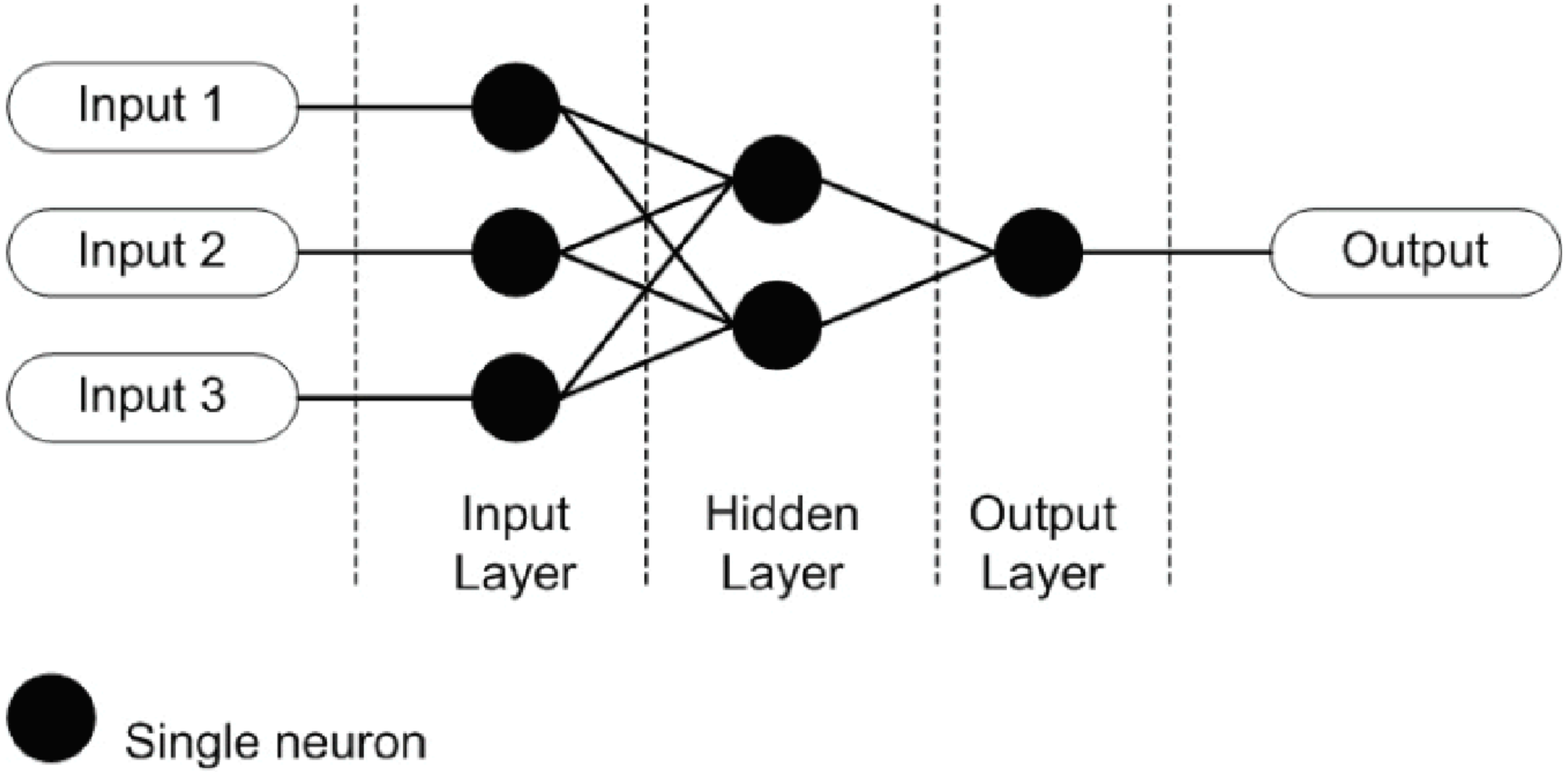
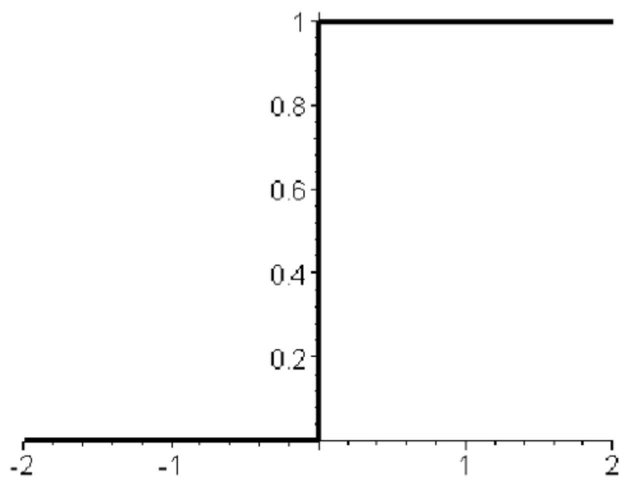
Combination of the Neurons yields NNs



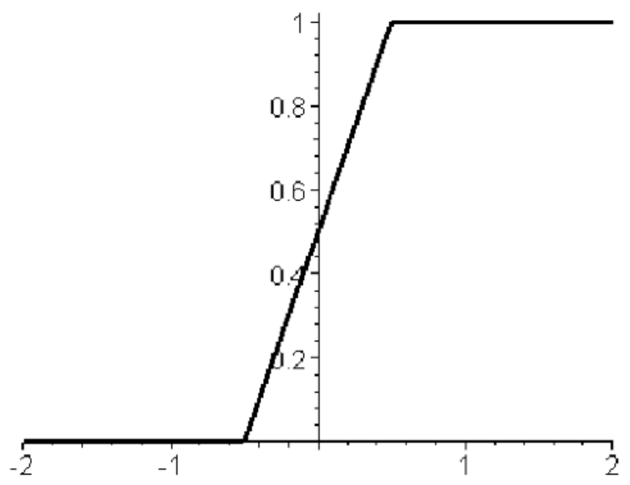
(1) *Threshold function*:

$$\varphi(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}$$



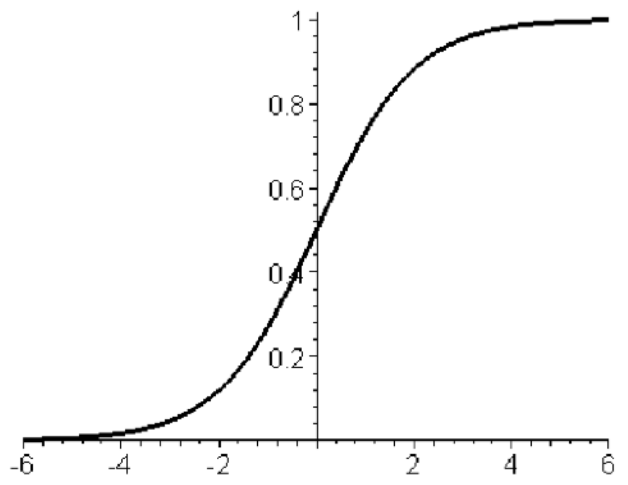
(2) *Piecewise linear function*:

$$\varphi(x) = \begin{cases} 1 & x \geq +\frac{1}{2} \\ x + \frac{1}{2} & \frac{1}{2} \geq x \geq -\frac{1}{2} \\ 0 & -\frac{1}{2} \geq x \end{cases}$$



(3) *Sigmoid function (logistic function)*:

$$\varphi(x) = \frac{1}{1 + e^{-x}}$$



Neural Net Training

Given is a continuous function

$$u : \Omega = [-1,1]^m \longrightarrow \mathbb{R}$$

that is sampled on a set $P \subseteq \Omega$.

Consider a neural net

$$\hat{u} : \Omega \times \Theta \longrightarrow \mathbb{R}\,, \quad \hat{u} = \hat{u}(x, W, B)$$

depending on x and weights & bias

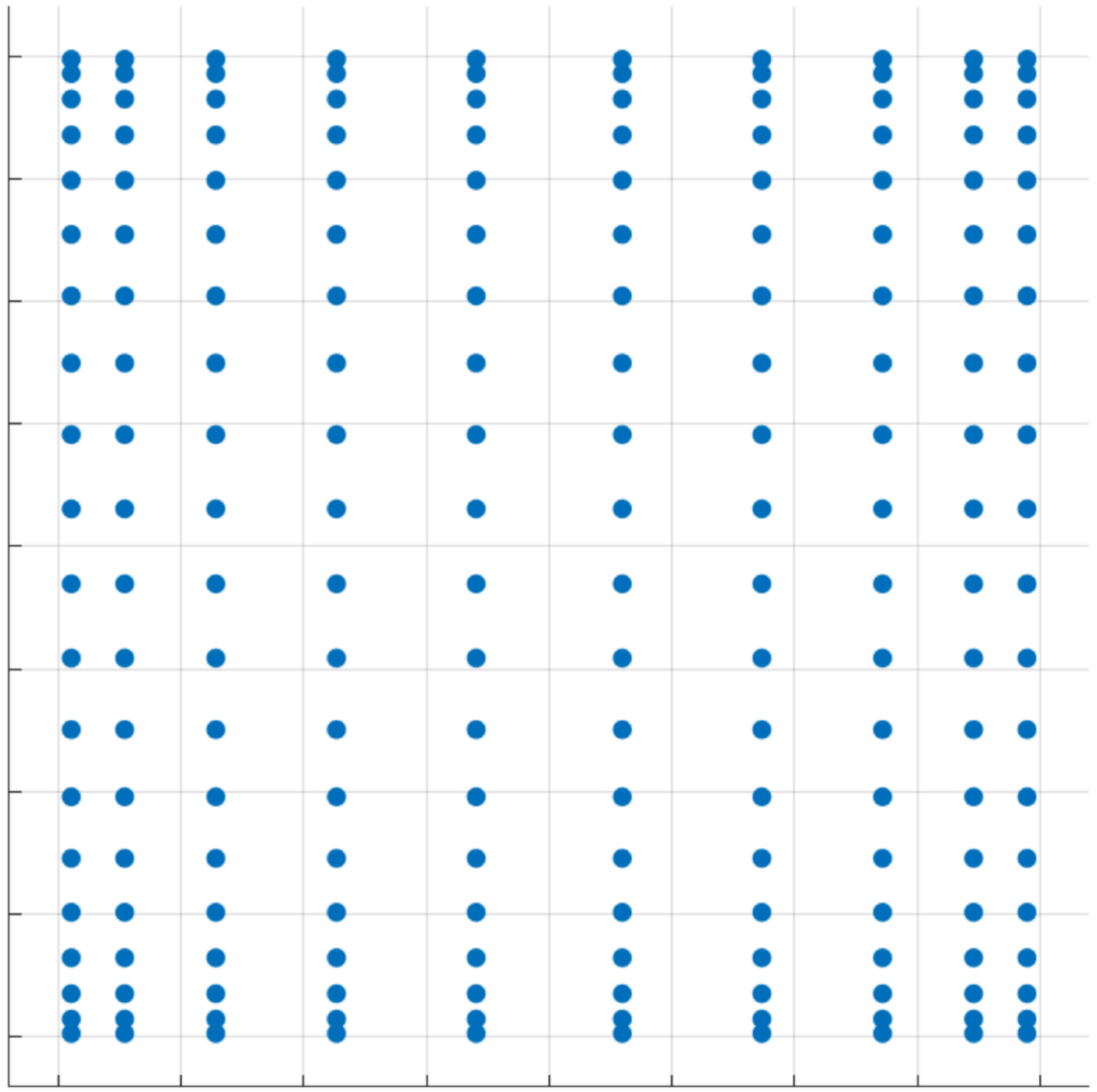
The mean square error (MSE) loss

$$\mathscr{L}(W,B) : \Theta \longrightarrow \mathbb{R}^+$$

is given by

$$\mathscr{L}(W,B) = \sum_{p \in P} \|u(p) - \hat{u}(p, W, B)\|^2 \approx \int_\Omega \|u(x) - \hat{u}(x, W, B)\|^2 d\Omega.$$

Loss approximations due to Gauss quadratures



Legendre grid in 2D

$$p_\alpha = (p_{\alpha_1}, \cdots, p_{\alpha_m}) \in G_{m,n}$$

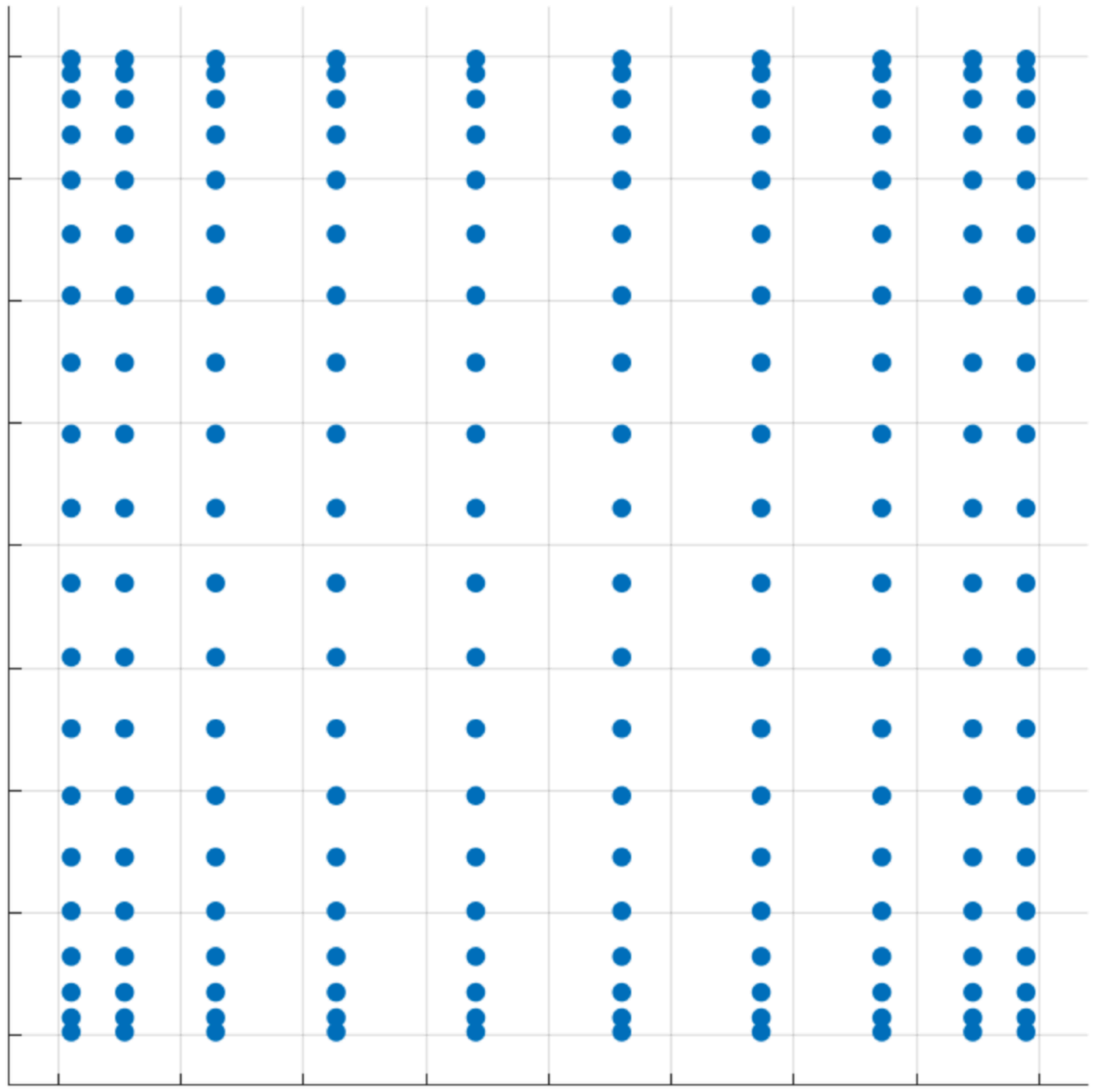
Lagrange polynomials in dimension $m \in \mathbb{N}$

$$A_{m,n} = \{\alpha \in \mathbb{N}^m : \|\alpha\|_1 \leq n\}$$

$$L_\alpha = \prod_{i=1}^{m} l_{\alpha_i,i}, \quad l_{j,i} = \prod_{h \neq j, h=0}^{n} \frac{x_i - p_h}{p_j - p_h}$$

$$L_\alpha(p_\beta) = \delta_{\alpha,\beta}$$

Loss approximations due to Gauss quadratures



Legendre grid in 2D

$$p_\alpha = (p_{\alpha_1}, \cdots, p_{\alpha_m}) \in G_{m,n}$$

Lagrange polynomials in dimension $m \in \mathbb{N}$

$$f(x) = \sum_{\alpha \in A_{m,n}} f(p_\alpha) L_\alpha = Q_{f,n}\,,$$

$$g(x) = \sum_{\alpha \in A_{m,n}} g(p_\alpha) L_\alpha = Q_{f,n}$$

$$\int_\Omega f(x)g(x)dx = \sum_{\alpha \in A_{m,n}} w_\alpha f(p_\alpha) g(p_\alpha)$$

w_α...Gauss-Legendre weights

Polynomial differentiation P.D.

Lagrange polynomials in dimension $m \in \mathbb{N}$

$$f(x) = \sum_{\alpha \in A_{m,n}} f(p_\alpha) L_\alpha = Q_{f,n}\,,$$

$$\partial^\alpha f(x) = \sum_{\alpha \in A_{m,n}} c_\alpha L_\alpha(x)\,, \quad C = (c_\alpha)_{\alpha \in A_{m,n}} = \mathbb{D}^\alpha F\,, F = (f(p_\alpha))_{\alpha \in A_{m,n}}$$

$\mathbb{D}^\alpha$...Polynomial Differential Operator

$$\mathbb{D}^\alpha = (\partial^\alpha L_\beta)_{\beta \in A_{m,n}} \in \mathbb{R}^{|A_{m,n}| \times |A_{m,n}|}\,, \quad \partial^\alpha L_\beta = \sum_{\gamma \in A_{m,n}} c_\gamma L_\gamma$$

Sobolev spaces

Sobolev spaces of regularity $k \in \mathbb{N}$

$$H^k(\Omega, \mathbb{R}) = \{f \in L^2(\Omega, \mathbb{R}) : \|\partial^\alpha f\|_{L^2(\Omega)} \leq \infty \, , \alpha \in \mathbb{N}^m \, , \|\alpha\|_1 \leq n\} \, ,$$

$$H^0(\Omega, \mathbb{R}) = L^2(\Omega, \mathbb{R})$$

$$\langle f, g \rangle_{H^k(\Omega)} = \sum_{\|\alpha\|_1 \leq n} \int_\Omega \partial^\alpha f(x) \partial^\alpha g(x) dx$$

Sobolev cubatures

Given polynomials $f(x) = \sum_{\alpha \in A_{m,n}} f(p_\alpha) L_\alpha = Q_{f,n}\,, g(x) = \sum_{\alpha \in A_{m,n}} g(p_\alpha) L_\alpha = Q_{f,n}$

$$\langle f, g \rangle_{H^k(\Omega)} = \sum_{\|\alpha\|_1 \leq n} (\mathbb{D}^\alpha F)^T W_{m,n} \mathbb{D}^\alpha G\,,$$

$$F = (f(p_\alpha))_{\alpha \in A_{m,n}}\,, G = (g(p_\alpha))_{\alpha \in A_{m,n}} \quad W_{m,n} = \mathrm{diag}(w_\alpha)_{\alpha \in A_{m,n}}$$

Loss Approximations

We are seeking for a smooth function solving a Poisson problem:

$\Delta u = 0$ **in** $\Omega = [-1,1]^m$

Poisson-PDE loss of neural nets with Automatic differentiation

$$\mathscr{L}(W,B) = \sum_{p \in P} \|\Delta \hat{u}(p,W,B)\|^2 \approx \int_\Omega \|\Delta \hat{u}(x,W,B)\|^2 d\Omega$$

Poisson-PDE loss of neural nets with Polynomial differentiation

$$\mathscr{L}(W,B) = (\mathbb{D}_\Delta \hat{U}(p_\alpha))^T W_{m,n} (\mathbb{D}_\Delta \hat{U}(p_\alpha)) \approx \|\Delta \hat{u}(x,W,B)\|^2_{L^2(\Omega)}.$$

$$\mathscr{L}(W,B) = \sum_{\|\beta\| \leq k} (\mathbb{D}^\beta \mathbb{D}_\Delta \hat{U}(p_\alpha))^T W_{m,n} \mathbb{D}_\Delta \mathbb{D}^\beta \hat{U}(p_\alpha)) \approx \|\Delta \hat{u}(x,W,B)\|^2_{H^k(\Omega)}$$

$\mathbb{D}_\Delta = \mathbb{D}^{2,0,\ldots,0} + \cdots + \mathbb{D}^{0,\cdots,0,2}$ **approximates the Laplacian**

Approximation Errors

Given a regular k-times differentiable function

$f : \Omega \longrightarrow \mathbb{R}$

Mean square error

$$\sum_{p \in P} \|f(p)\|^2 - \int_\Omega \|f(x)\|^2 d\Omega \in \mathcal{O}\left(\frac{1}{\sqrt{|P|}}\right)$$

Gauss cubature error

$$F^T W_{m,n} F - \int_\Omega \|f(x)\|^2 d\Omega \in \mathcal{O}\left(\frac{1}{k(n-k)^k}\right), \quad |A_{m,n}| = (n+1)^m$$

In low dimensions Gauss quadrature is more powerful than Monte Carlo integration !

Runtime Complexity

Theorem 4. *For a given deep Neural Network $\hat{u}_\theta : \Omega \to \mathbb{R}$, with architecture $\xi_{m,1}$ consisting of l hidden layers and q neurons per layer, the complexity per epoch for computing the $k-$th derivative $(\partial_x^k \hat{u}_\theta)$ in $s \in \mathbb{N}$ training points is given by*

i) $\mathcal{O}(2^{k-1} lsq^2)$ *for a PINN resting on A.D., i.e. it scales exponentially with the order of the derivative.*

ii) $\mathcal{O}(\max\{s^2, lsq^2\})$ *for the SC-PINN using P.D.*

In low dimensions $m \leq 4$ Polynomial Differentiation (P.D.) is faster than Automatic Differentiation (A.D.) !

Cardona, J. E. S., & Hecht, M. (2022). Replacing Automatic Differentiation by Sobolev Cubatures fastens Physics Informed Neural Nets and strengthens their Approximation Power. *arXiv preprint arXiv:2211.15443*.

Examples

We start by addressing the Poisson problem in dimension $m = 2$

$$\begin{cases} -\Delta u(x) - f(x) &= 0 \quad , \forall x \in \Omega = [-1,1]^2 \\ u(x) - g(x) &= 0 \quad , \forall x \in \partial\Omega \,, \end{cases} \tag{30}$$

described in detail Eq. (11). We choose $f(x,y) := -2\lambda^2 \cos(\lambda x)\sin(\lambda y)$ and $g(x) := \cos(\lambda x)\sin(\lambda y)$, with frequency $\lambda = 2\pi q$, $q = 6$, yielding $u(x,y) = g(x,y)$ to be the analytic solution.

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Examples

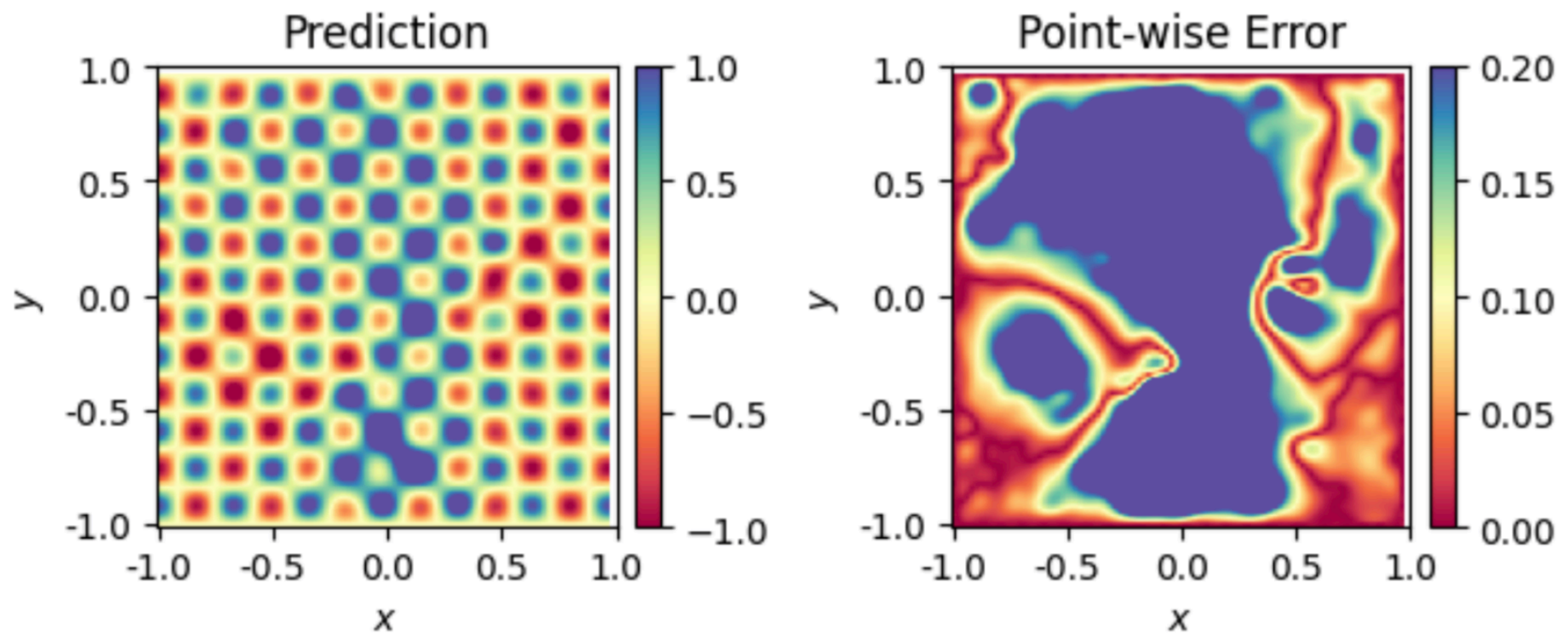

Figure 1. ID-PINN with MSE loss, reaching $\epsilon_\infty = 1.24$, $\epsilon_1 = 2.22\text{e-}1$, $t \approx 1173$.

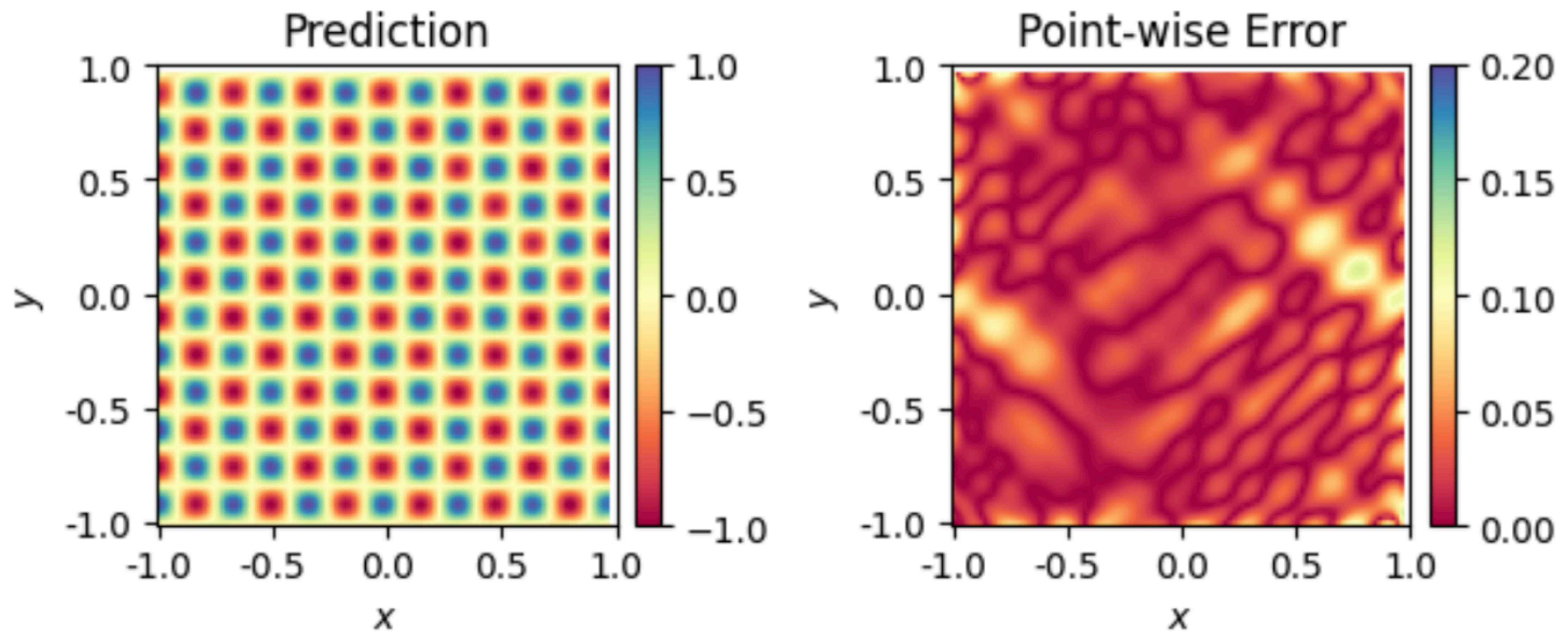

Figure 2. SC-PINN with strong Sobolev loss and A.D., reaching $\epsilon_\infty = 1.37\text{e-}1$, $\epsilon_1 = 2.27\text{e-}2$, $t \approx 725$.

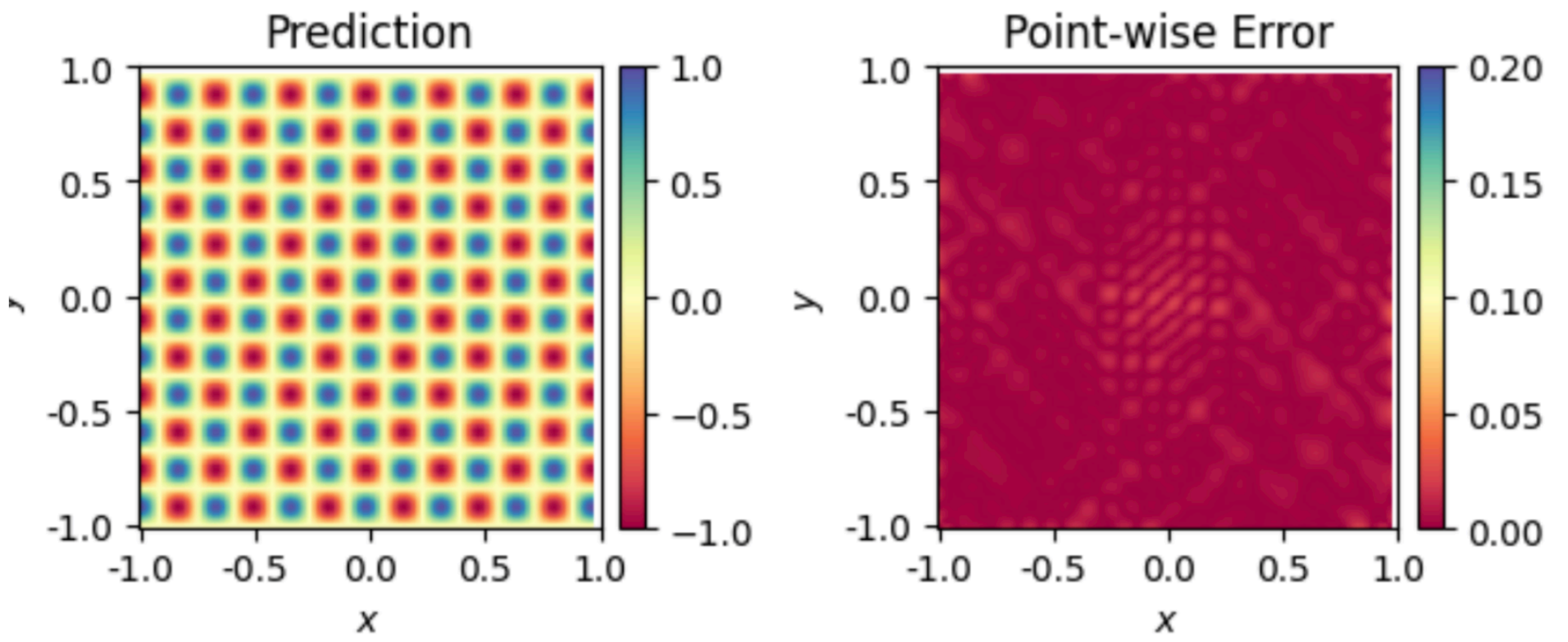

Figure 3. SC-PINN with strong Sobolev loss and P.D., reaching $\epsilon_\infty = 3.00\text{e-}2$, $\epsilon_1 = 3.75\text{e-}3$, $t \approx 192$.

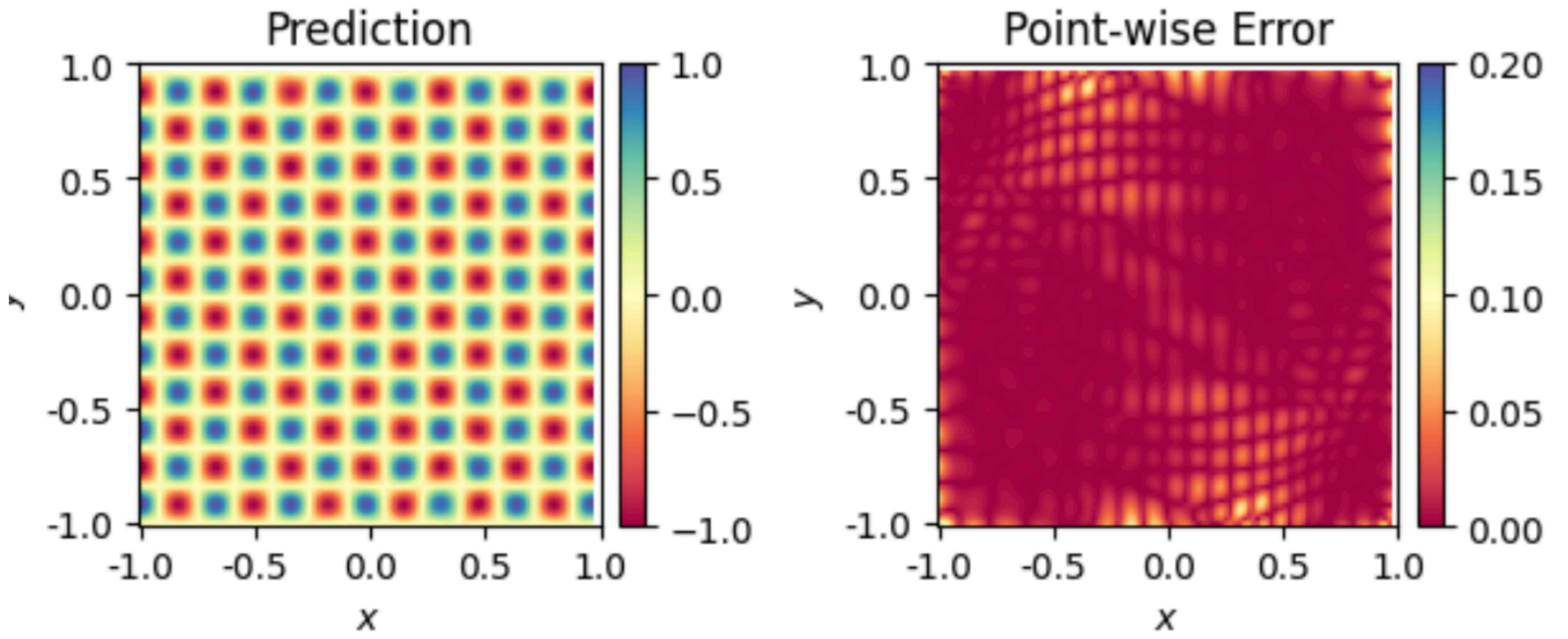

Figure 4. SC-PINN with strong variational Sobolev loss and P.D., reaching $\epsilon_\infty = 1.25\text{e-}1$, $\epsilon_1 = 7.70\text{e-}3$, $t \approx 188$.

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Examples

The time independent *Quantum Harmonic Oscillator* in dimension $m = 2$, corresponds to the *Schrödinger equation* with the linear potential $V(u(x)) := (x_1^2 + x_2^2)u(x)$, $u \in C^2(\Omega, \mathbb{R})$, see e.g. (Griffiths and Schroeter, 2018; Liboff, 1980), given by:

$$\begin{cases} -\Delta u(x) + V(u(x)) &= \lambda u(x) \quad ,\forall x \in \Omega \\ u(x) - g(x) &= 0 \quad ,\forall x \in \partial\Omega\,, \end{cases} \tag{31}$$

We consider the eigenvalue problem $\lambda = n_1 + n_2 + 1$, $n_1, n_2 \in \mathbb{N}$ with eigenfunctions

$$g(x_1, x_2) = \frac{\pi^{-1/4}}{\sqrt{2^{n_1+n_2} n_1! n_2!}} e^{-\frac{(x_1^2+x_2^2)}{2}} H_{n_1}(x_1) H_{n_2}(x_2)\,,$$

We choose $\lambda = 15$

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Examples

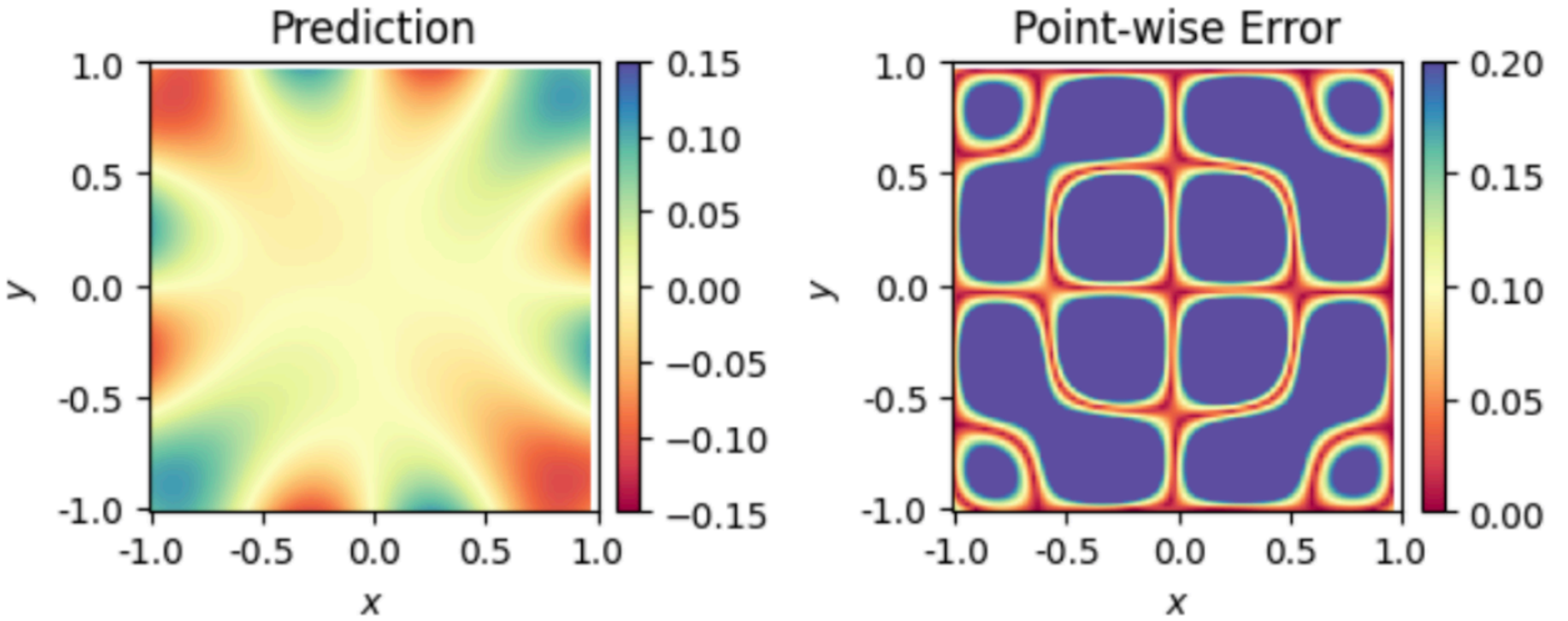

Figure 5. ID-PINN with MSE loss and A.D., reaching $\epsilon_\infty = 1.46\text{e-}1$, $\epsilon_1 = 4.78\text{e-}2$, $t \approx 905$,

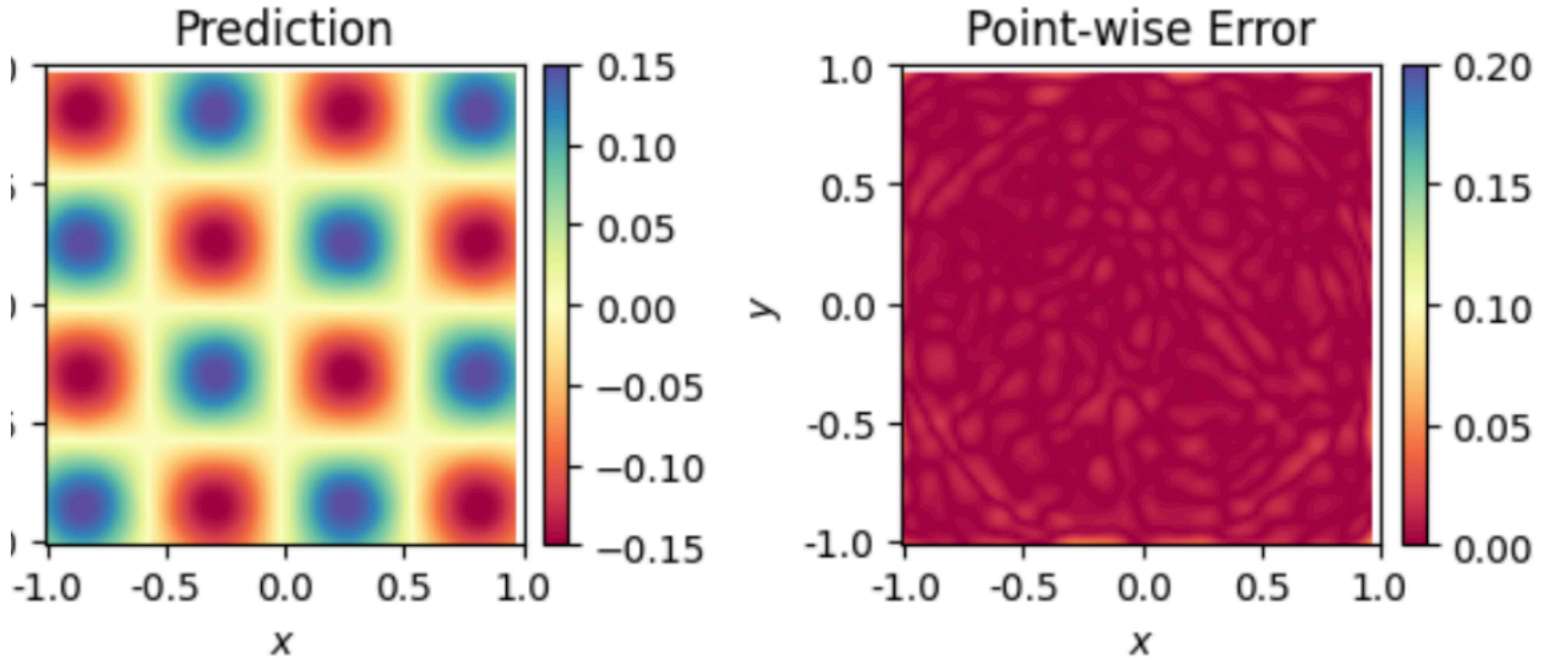

Figure 7. SC-PINN with strong variational Sobolev loss and P.D., reaching, $\epsilon_\infty = 7.27\text{e-}3, \epsilon_1 = 8.16\text{e-}4, t \approx 167$,

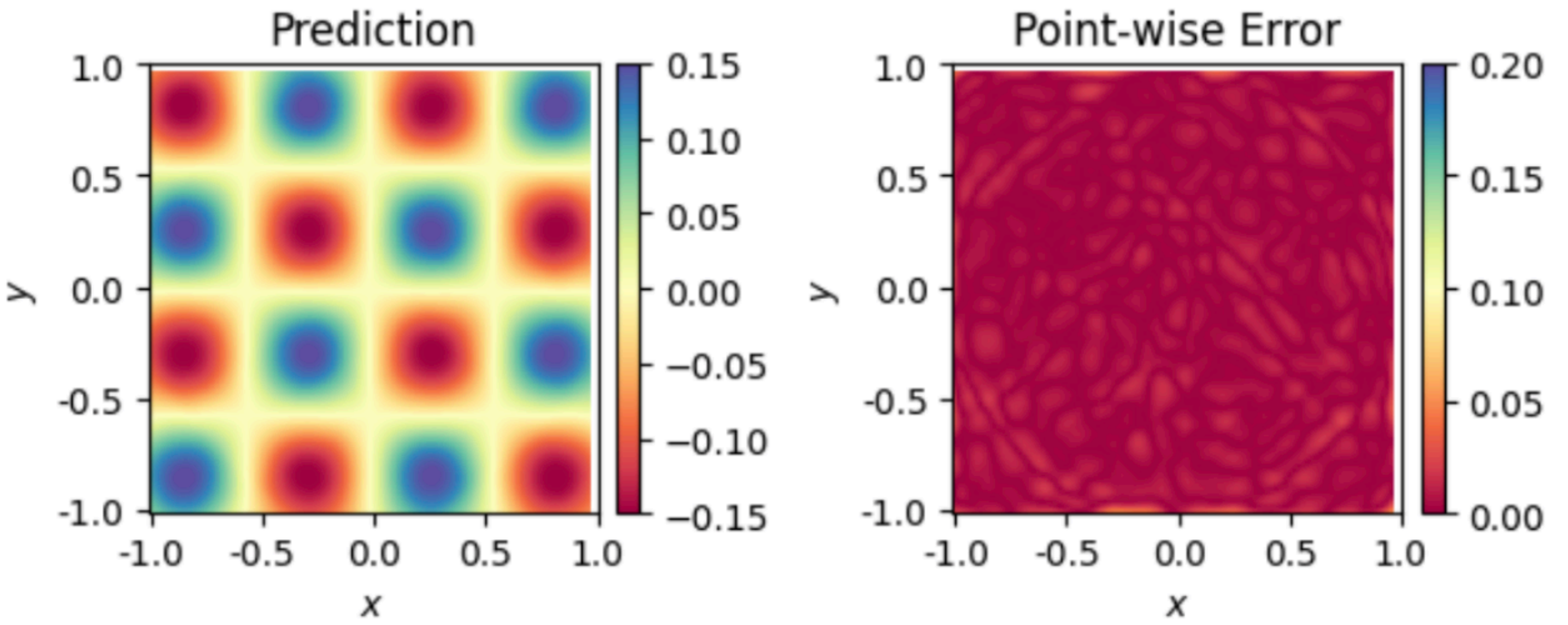

Figure 6. SC-PINN with strong Sobolev loss and P.D., reaching, $\epsilon_\infty = 1.22\text{e-}2$, $\epsilon_1 = 1.24\text{e-}3$, $t \approx 165$,

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Examples

We re-investigate PINN-solutions of the Poisson problem in dimension $m = 1$, whose analytic solutions include hard transitions. That is, choosing

$$f(x) := C\left(A\omega^2 \sin(\omega x) + 2\beta^2 \text{sech}^2(x) \tanh(\beta x)\right),$$

with boundary condition $g(x) := C(A \sin(\omega x) + \tanh(\beta x))$ yielding $u(x) = g(x)$ to be the analytic solution. Two scenarios were considered:

$$S_1 = \{C = 0.1, A = 0.1, \beta = 30, \omega = 20\pi, \text{bs} = 100\}$$
$$S_2 = \{C = 0.1, A = 0.1, \beta = 5, \omega = 26.5\pi, \text{bs} = 100\}$$

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Examples

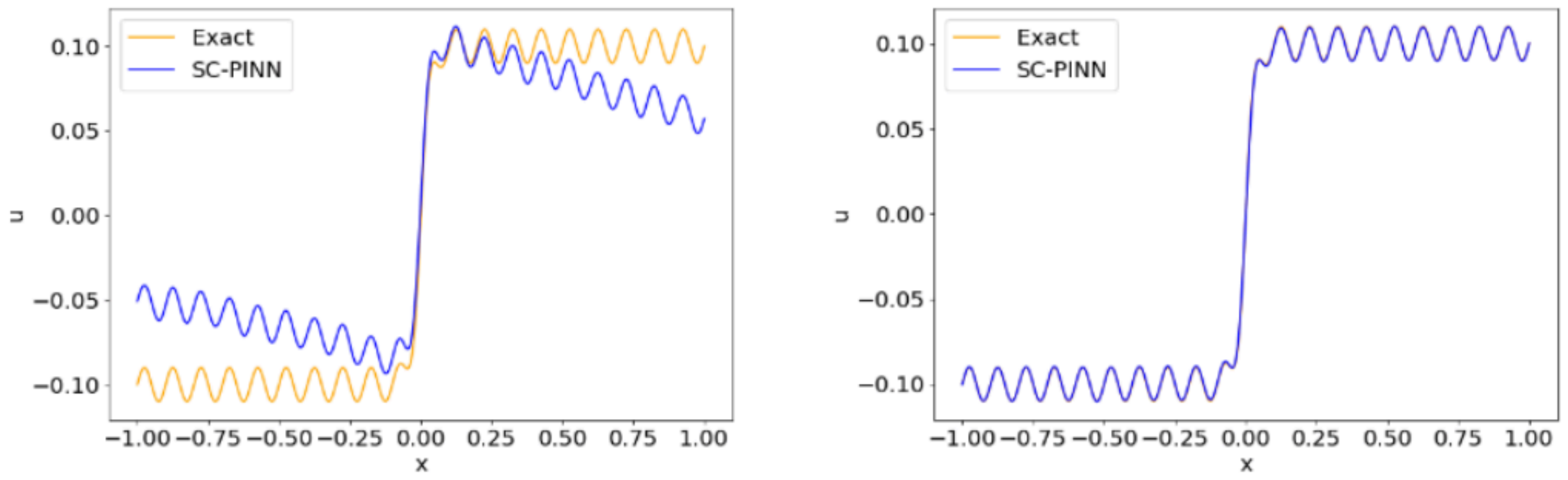

Figure 8. SC-PINN with strong Sobolev loss and P.D. (left), reaching $\epsilon_\infty = 3.04e-2$, $\epsilon_1 = 7.24e-2, t \approx 150$, SC-PINN with strong variational Sobolev loss and P.D.(right), reaching $\epsilon_\infty = 2.0\text{e-}3$, $\epsilon_1 = 4.0\text{e-}4, t \approx 151$, scenario S_1.

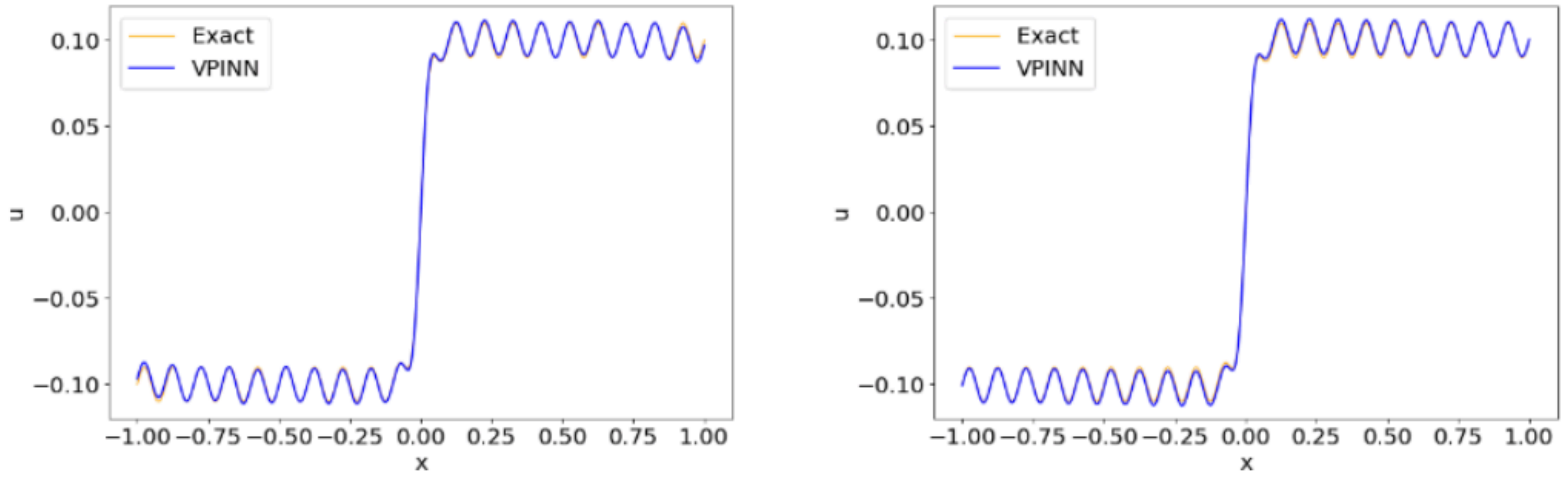

Figure 9. VPINN with $N_{\text{el}} = 1$ (left), reaching $\epsilon_\infty = 3.29\text{e-}3$, $\epsilon_1 = 9.94\text{e-}4, t \approx 96$, VPINN with $N_{\text{el}} = 3$ (right), reaching $\epsilon_\infty = 2.73\text{e-}3$, $\epsilon_1 = 1.40\text{e-}3, t \approx 191$, scenario S_1.

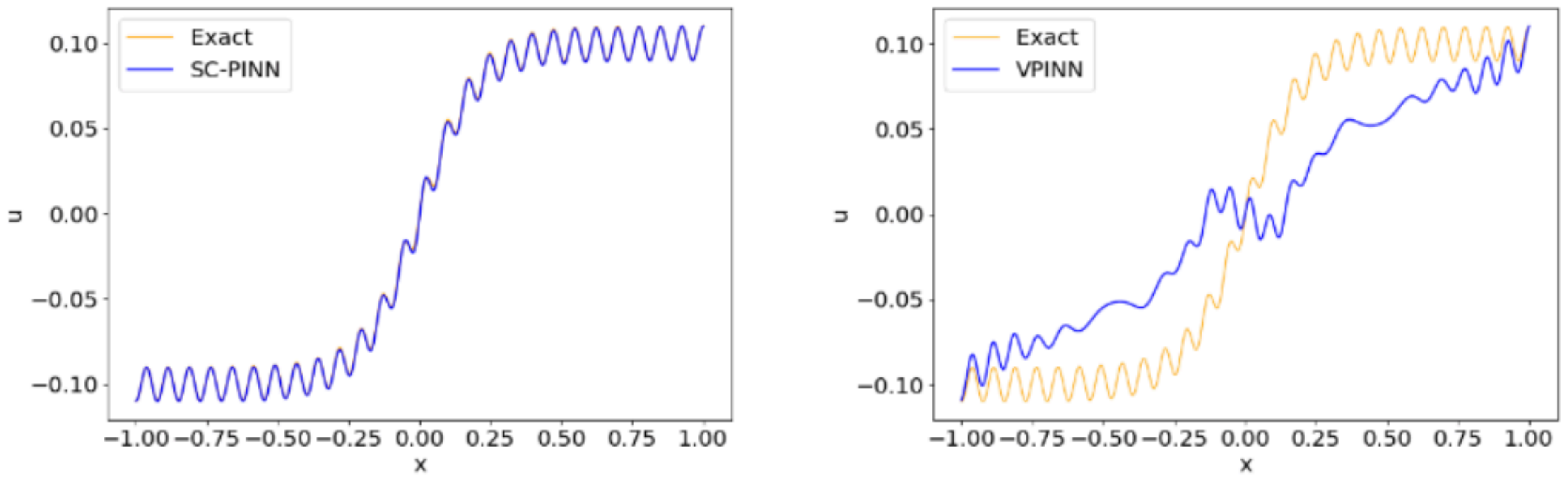

Figure 10. SC-PINN with strong variational Sobolev loss and P.D.(left), reaching $\epsilon_\infty = 2.75\text{e-}3$, $\epsilon_1 = 5.35\text{e-}4, t \approx 151$, VPINN with $N_{\text{el}} = 3$, reaching $\epsilon_\infty = 6.50\text{e-}2$, $\epsilon_1 = 3.40\text{e-}2$, scenario S_2, $t \approx 180$.

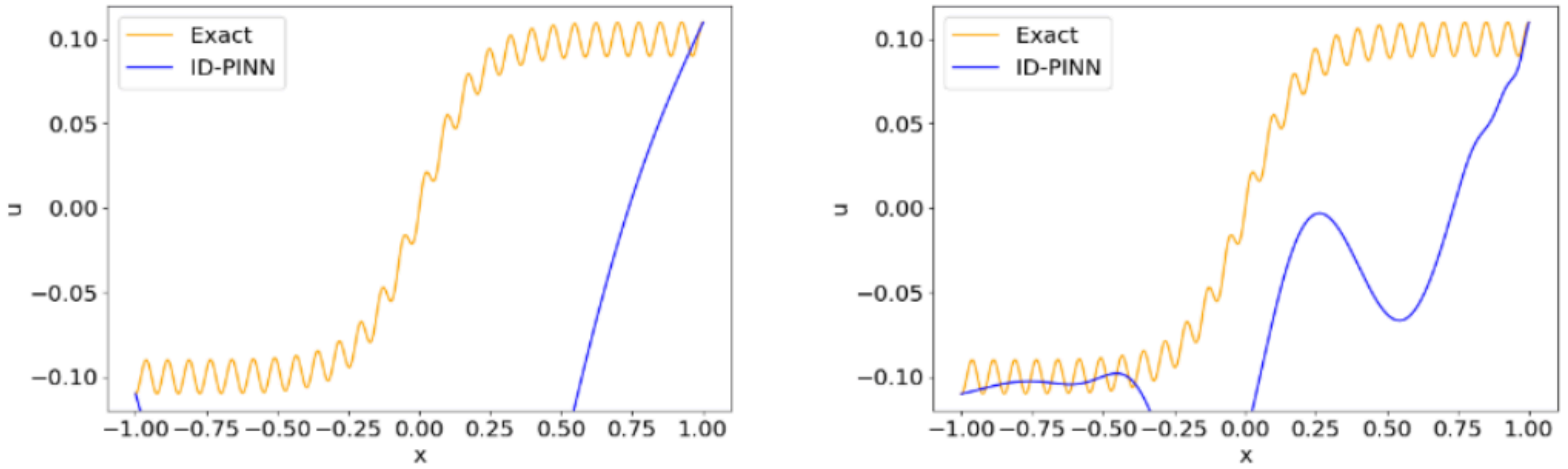

Figure 11. ID-PINN with MSE loss, bs = 500 and A.D.,(left), reaching $\epsilon_\infty = 4.74\text{e-}1$, $\epsilon_1 = 2.50\text{e-}1, t \approx 158$, ID-PINN with MSE loss without I.D., bs = 5000 and A.D.,(right), reaching $\epsilon_\infty = 1.73\text{e-}1$, $\epsilon_1 = 7.13\text{e-}2, t \approx 360$, scenario S_2.

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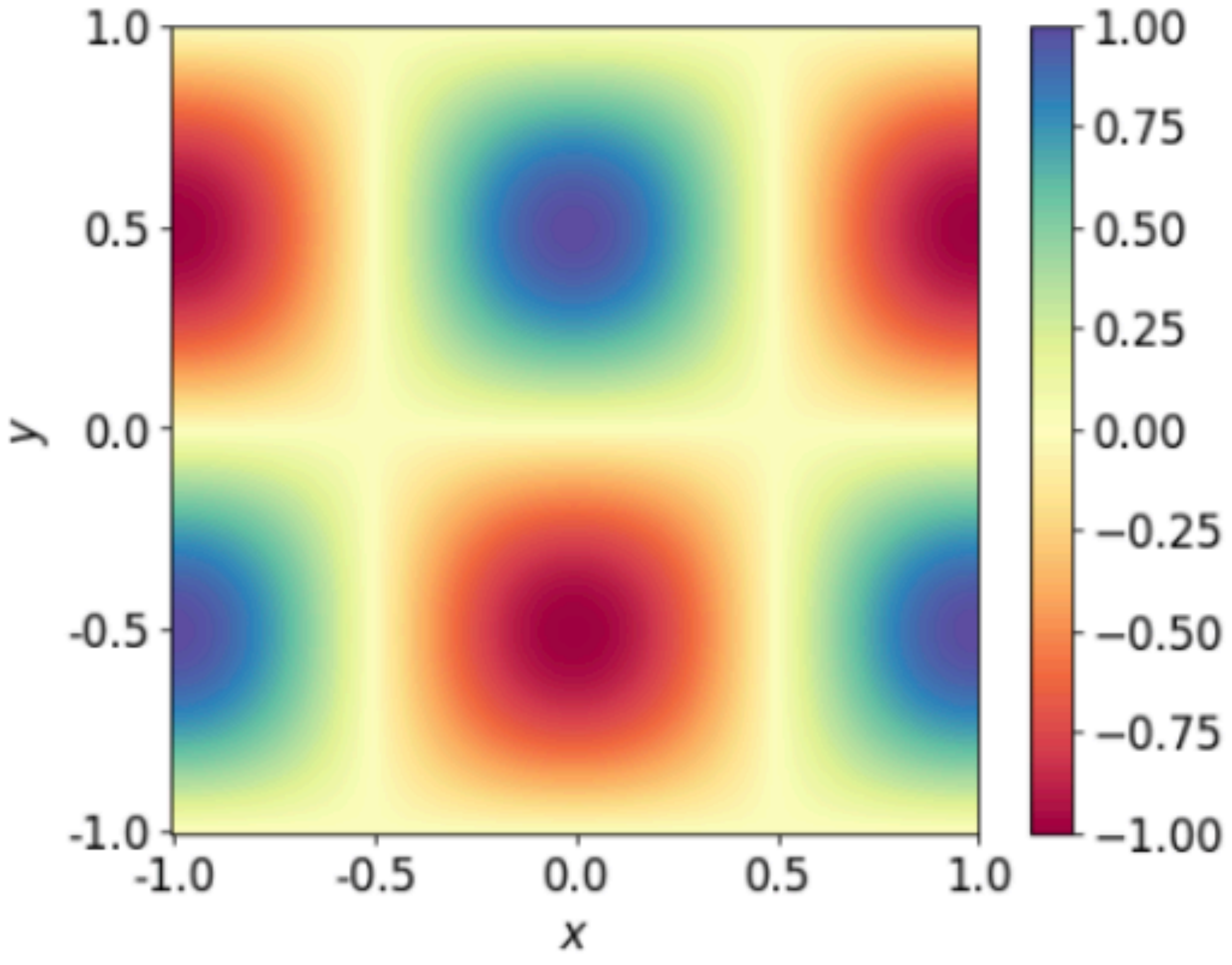
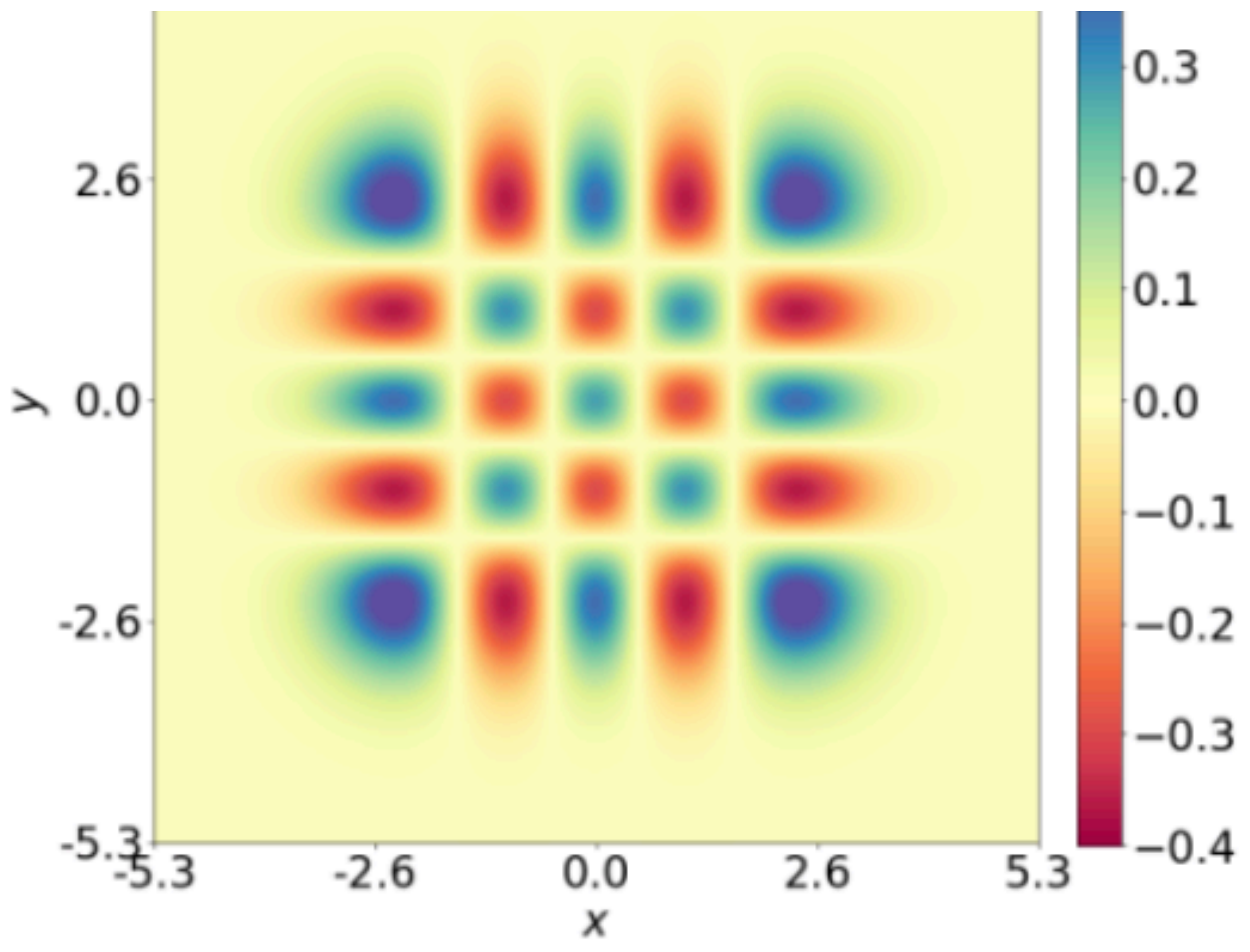
Inverse Eigenvalue Problems



Method	Approximation error		Runtime (s)
	ϵ_λ	ϵ_1	
PINN	$4.63 \cdot 10^{-1}$	$1.13 \cdot 10^{-2}$	$t \approx 1592$
ID-PINN	$2.14 \cdot 10^{-2}$	$8.09 \cdot 10^{-4}$	$t \approx 2184$
SC-PINN	$\mathbf{3 \cdot 10^{-4}}$	$\mathbf{5.49 \cdot 10^{-4}}$	$t \approx \mathbf{103}$

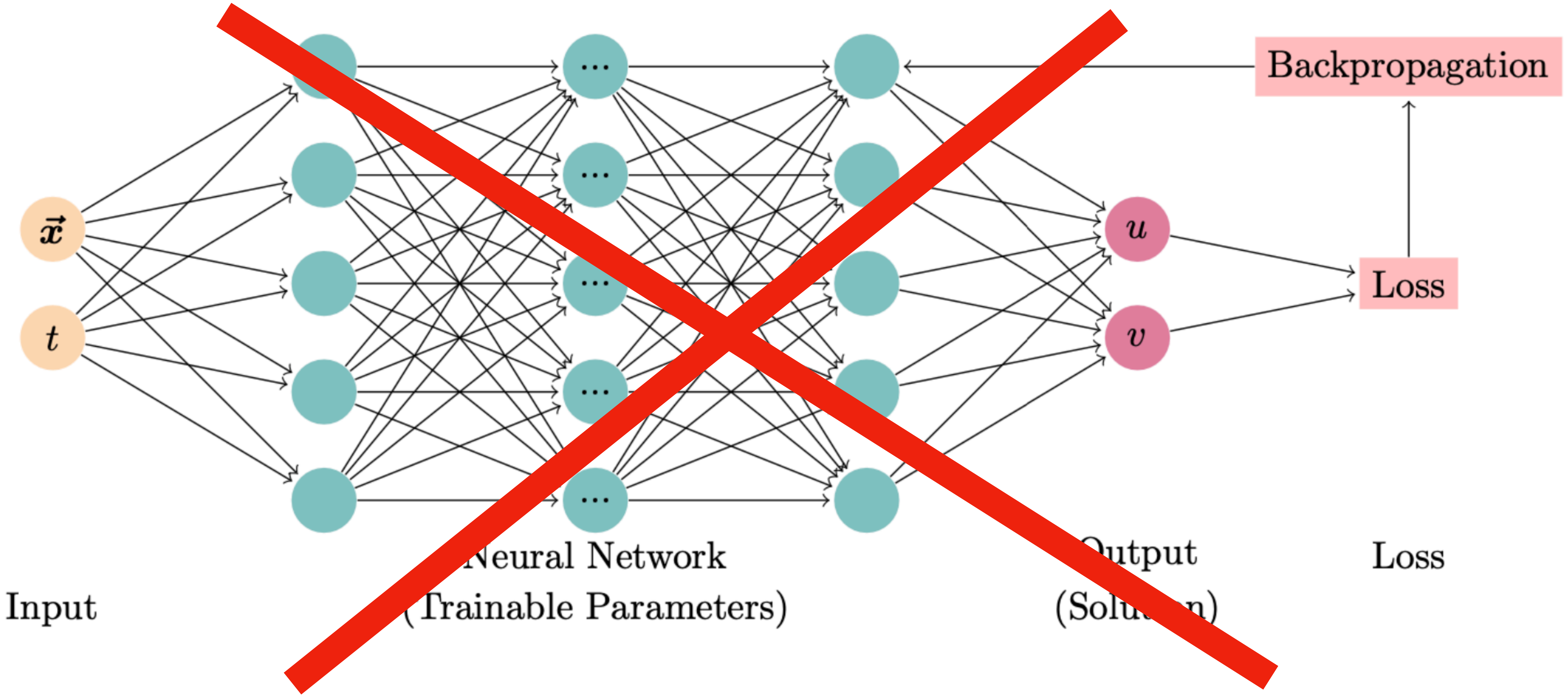
Figure 12. Solution and errors for 2D Poisson inverse problem with $\lambda_{gt} = \pi$.



Method	Approximation error		Runtime (s)
	ϵ_λ	ϵ_1	
PINN	6.01	$7.32 \cdot 10^{-2}$	$t \approx 1414$
ID-PINN	$6.21 \cdot 10^{-2}$	$7.51 \cdot 10^{-3}$	$t \approx 1346$
SC-PINN	$\mathbf{2.18 \cdot 10^{-4}}$	$\mathbf{5.68 \cdot 10^{-4}}$	$t \approx \mathbf{192}$

Figure 13. Solution and errors for 2D QHO inverse problem with $\lambda_{gt} = 5$.

Replace the Neural Net by (Spectral) Polynomial Surrogate Models (e.g. Chebyshev Polynomials)



$$\hat{u}(x,\Theta) = \sum_{\alpha \in A_{m,n}} \theta_\alpha T_\alpha(x)\,, \quad \Theta = (\theta_\alpha)_{\alpha \in A_{m,n}} \in \mathbb{R}^{|A_{m,n}|}$$

$$T_\alpha(\cos(x)) = T_\alpha(\cos(x_1),\ldots,\cos(x_m)) = \prod_{i=1}^{m} \cos(\alpha_i x_i) = \cos(\alpha x)$$

(Spectral) Polynomial Surrogates Models (PSMs)
(Work in Progress)

$$\hat{u}(x,\Theta) = \sum_{\alpha \in A_{m,n}} \theta_\alpha T_\alpha(x)\,, \quad \Theta = (\theta_\alpha)_{\alpha \in A_{m,n}} \in \mathbb{R}^{|A_{m,n}|}$$

$$T_\alpha(\cos(x)) = T_\alpha(\cos(x_1),\dots,\cos(x_m)) = \prod_{i=1}^{m} \cos(\alpha_i x_i) = \cos(\alpha x)$$

Formulate losses with respect to Sobolev spaces of negative order

$$H^{-k}(\Omega,\mathbb{R}) := \overline{\mathscr{D}}^{\|\cdot\|_{H^{-k}(\Omega)}}\,, \quad \|F\|_{H^{-k}(\Omega)} = \sup_{u \in H^k(\Omega,\mathbb{R})} \frac{|Fu|}{\|u\|_{H^k(\Omega)}}$$

(Spectral) Polynomial Surrogates Models (PSMs)
(Work in Progress)

Experiment 4.1 (Non-periodic 2D-Poisson forward problem with hard transitions). *We consider the Poisson equation with right hand side function f given by*

$$
\begin{aligned}
f(x,y) =& C(A\sin(\omega y)+\tanh(\beta y))(-A\omega^2\sin(\omega x)-2\beta^2\tanh(\beta x)\mathrm{sech}^2(\beta x)) \\
&+C(A\sin(\omega x)+\tanh(\beta x))(-A\omega^2\sin(\omega y)-2\beta^2\tanh(\beta y)\mathrm{sech}^2(\beta y)),
\end{aligned}
$$

with $C=0.1, A=0.1, \beta=5, \omega=10\pi$. All the experiments where conducted with the same number of training points, as required for the Sobolev cubatures of degree $n=50$ in the domain and $n=100$ for the boundary. For the SC-PINN the weak L^2 -loss was used for the PDE loss and for the boundary one.

(Spectral) Polynomial Surrogates Models (PSMs)
(Work in Progress)

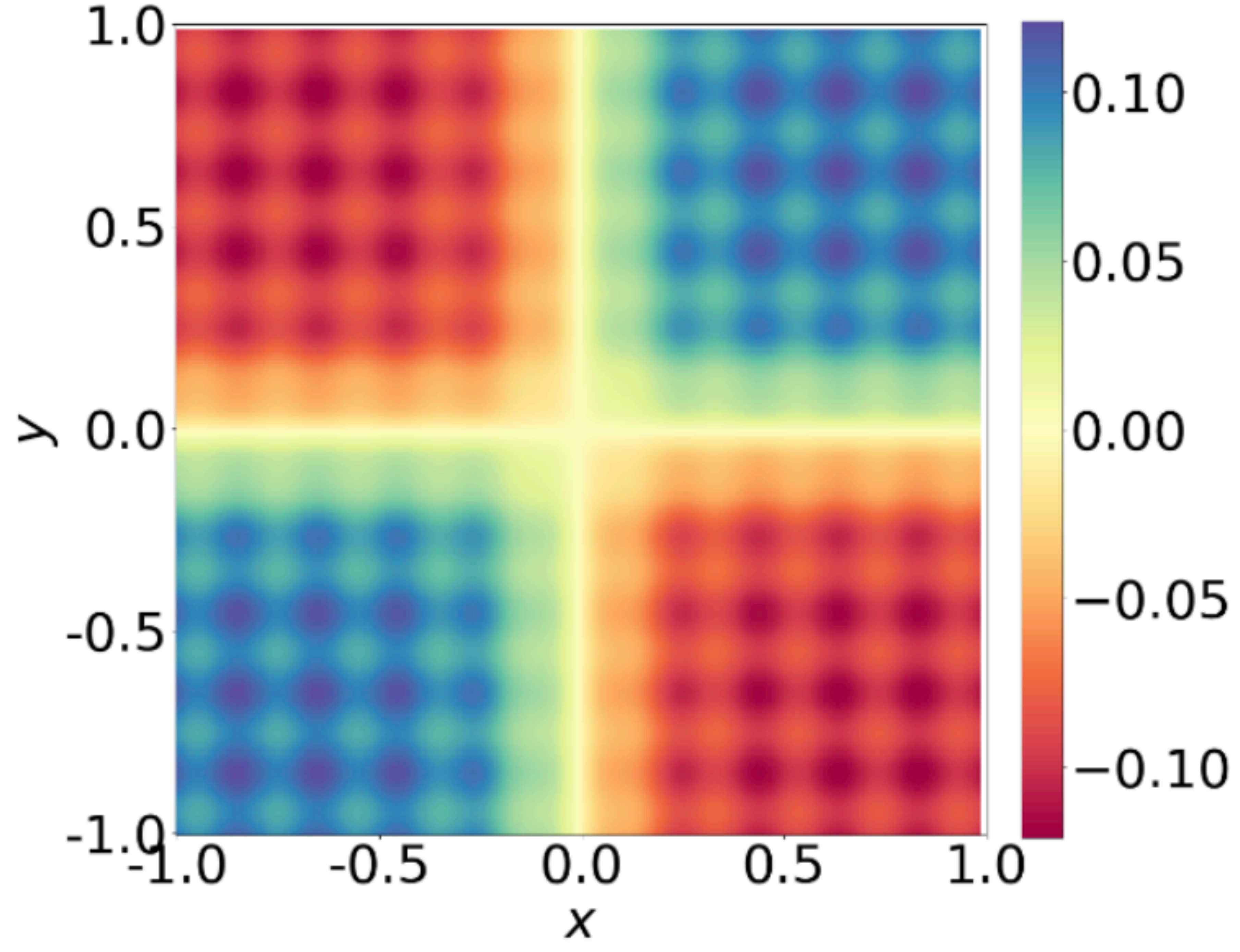


Figure 1: Solution for 2D Poisson problem

	Approximation error		Runtime (s)
dim = 2	ϵ_1	ϵ_∞	
PINN	$4.43 \cdot 10^{-3}$	$5.2 \cdot 10^{-2}$	$t = 886$
ID-PINN	$5.23 \cdot 10^{-3}$	$1.9 \cdot 10^{-2}$	$t = 1356$
SC-PINN	$2.52 \cdot 10^{-3}$	$3.33 \cdot 10^{-2}$	$t = 79.2$
GF-PSM	$5.37 \cdot 10^{-5}$	$2.94 \cdot 10^{-3}$	$t = 12.84$
AD-PSM	$\mathbf{8.79 \cdot 10^{-10}}$	$\mathbf{1.25 \cdot 10^{-8}}$	$\mathbf{t = 1.21}$

	Approximation error		Runtime (s)
dim = 4	ϵ_1	ϵ_∞	
GF-PSM	$1.33 \cdot 10^{-6}$	$1.0 \cdot 10^{-3}$	$t = 173.59s$
AD-PSM	$\mathbf{5.42 \cdot 10^{-8}}$	$\mathbf{6.37 \cdot 10^{-7}}$	$t = \mathbf{7.66s}$

Table 1: Errors for 2D and 4D Poisson forward problem

Poisson Inverse Eigenvalue Problem

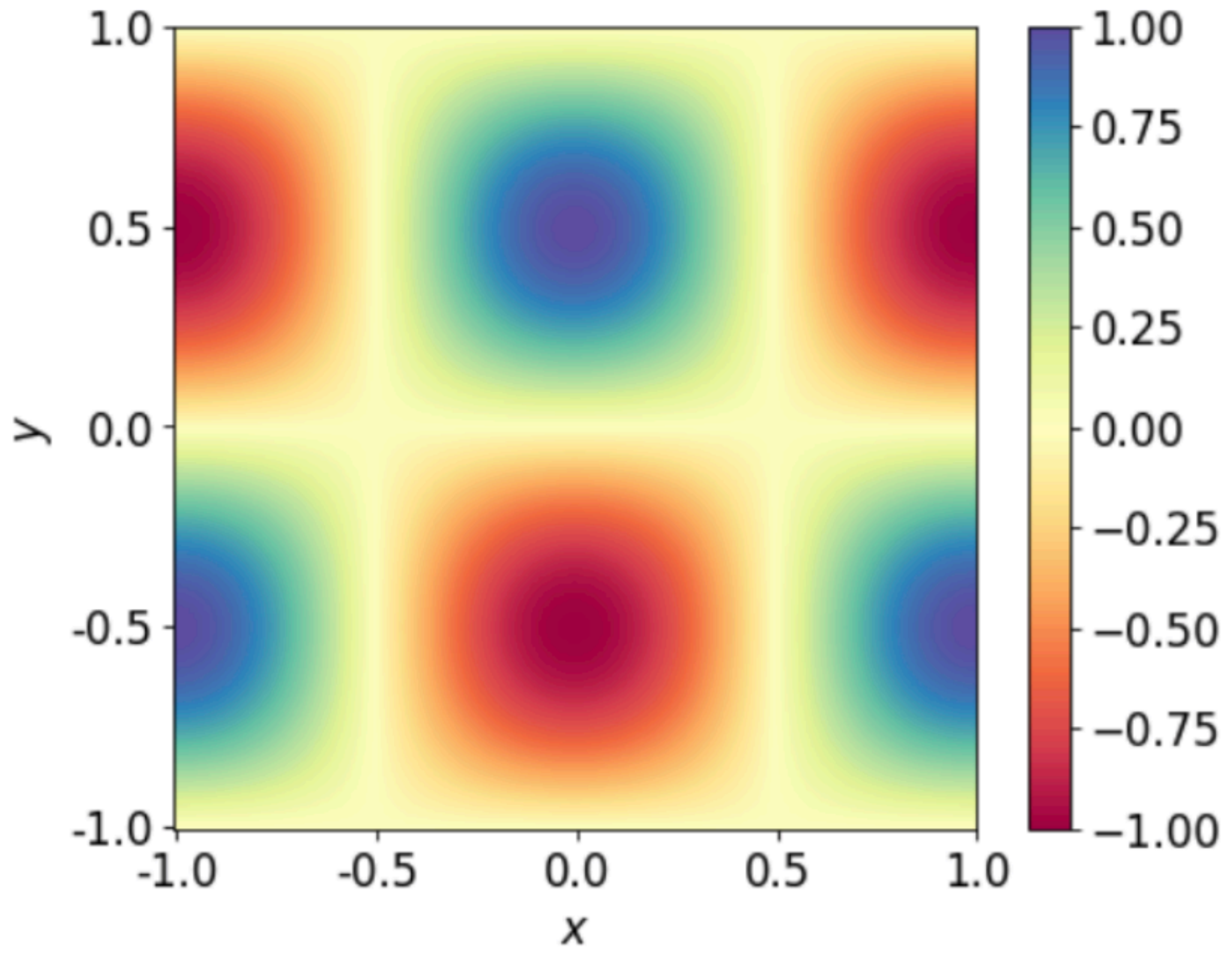


Figure 2: Solution for 2D inverse Poisson problem with $\omega_{gt} = \pi$.

	Approximation error		Runtime (s)
	ϵ_λ	ϵ_1	
PINN	$4.63 \cdot 10^{-1}$	$1.13 \cdot 10^{-2}$	$t \approx 1592$
ID-PINN	$2.14 \cdot 10^{-2}$	$8.09 \cdot 10^{-4}$	$t \approx 2184$
SC-PINN	$3 \cdot 10^{-4}$	$5.49 \cdot 10^{-4}$	$t \approx 103$
GF-PSM	$\mathbf{5.8 \cdot 10^{-8}}$	$\mathbf{6.0 \cdot 10^{-10}}$	$t \approx \mathbf{0.49}$

Table 2: Errors for 2D Poisson inverse problem

Quantum Harmonic Oscillator (QHO) forward Problem

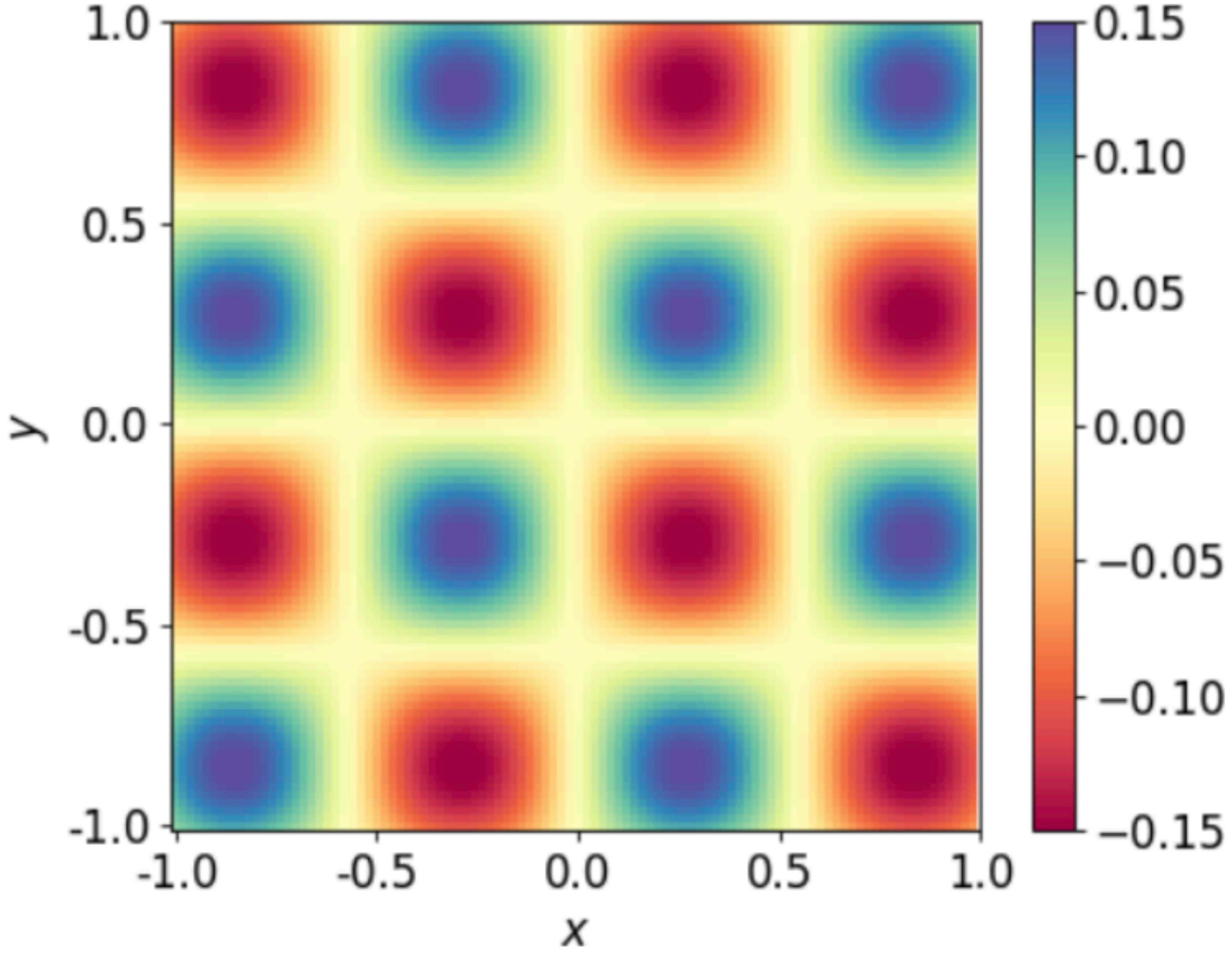


Figure 3: Solution of 2D QHO forward problem with $\mu = 21$.

	Approximation error		Runtime (s)
$\mu = 21$	ϵ_1	ϵ_∞	
PINN	$6.97 \cdot 10^{-2}$	$1. \cdot 10^{-3}$	$t \approx 776$
ID-PINN	$4.29 \cdot 10^{-2}$	$1.30 \cdot 10^{-1}$	$t \approx 948$
SC-PINN	$8.16 \cdot 10^{-4}$	$7.27 \cdot 10^{-3}$	$t \approx 167$
GF-PSM	$1.6 \cdot 10^{-8}$	$5.4 \cdot 10^{-8}$	$t \approx 0.16$
AD-PSM	$\mathbf{7.61 \cdot 10^{-13}}$	$\mathbf{2.37 \cdot 10^{-12}}$	$t \approx \mathbf{0.07}$
$\mu = 31$	ϵ_1	ϵ_∞	
GF-PSM	$1.09 \cdot 10^{-9}$	$1.45 \cdot 10^{-8}$	$t \approx 2.39$
AD-PSM	$\mathbf{2.25 \cdot 10^{-9}}$	$\mathbf{9.82 \cdot 10^{-9}}$	$t \approx \mathbf{1.07}$

Table 3: Errors for 2D QHO forward problem with $\mu = 21, 31$.

QHO forward Problem

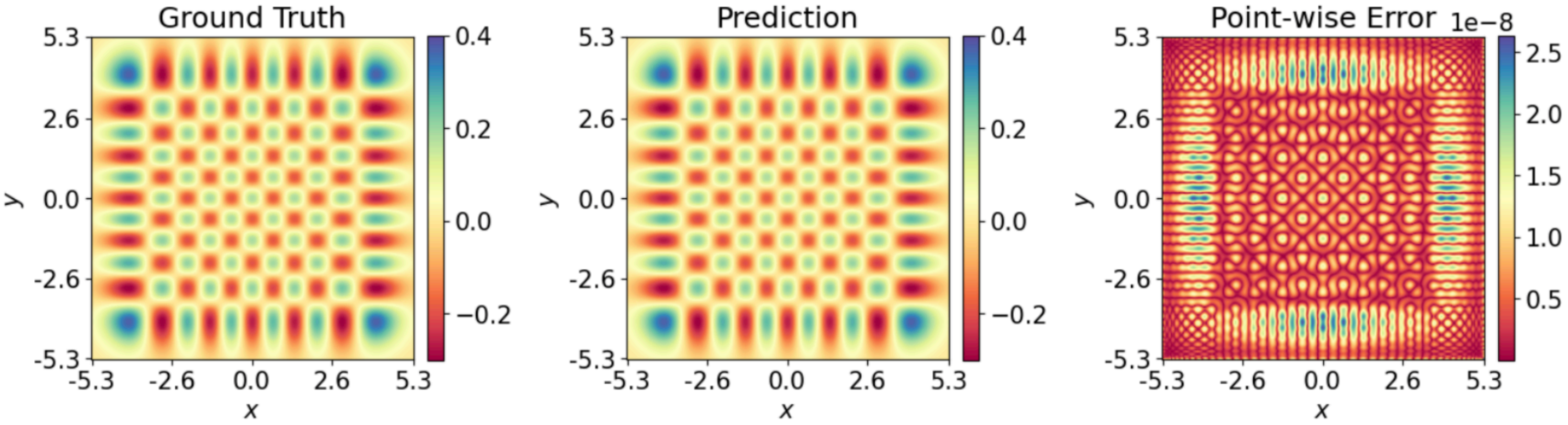


Figure 4: Solution for 2D QHO with $\mu = 31$ on $\Omega' = 5.3\Omega$ due to AD-PSM.

QHO Eigenvalue Inverse Problem

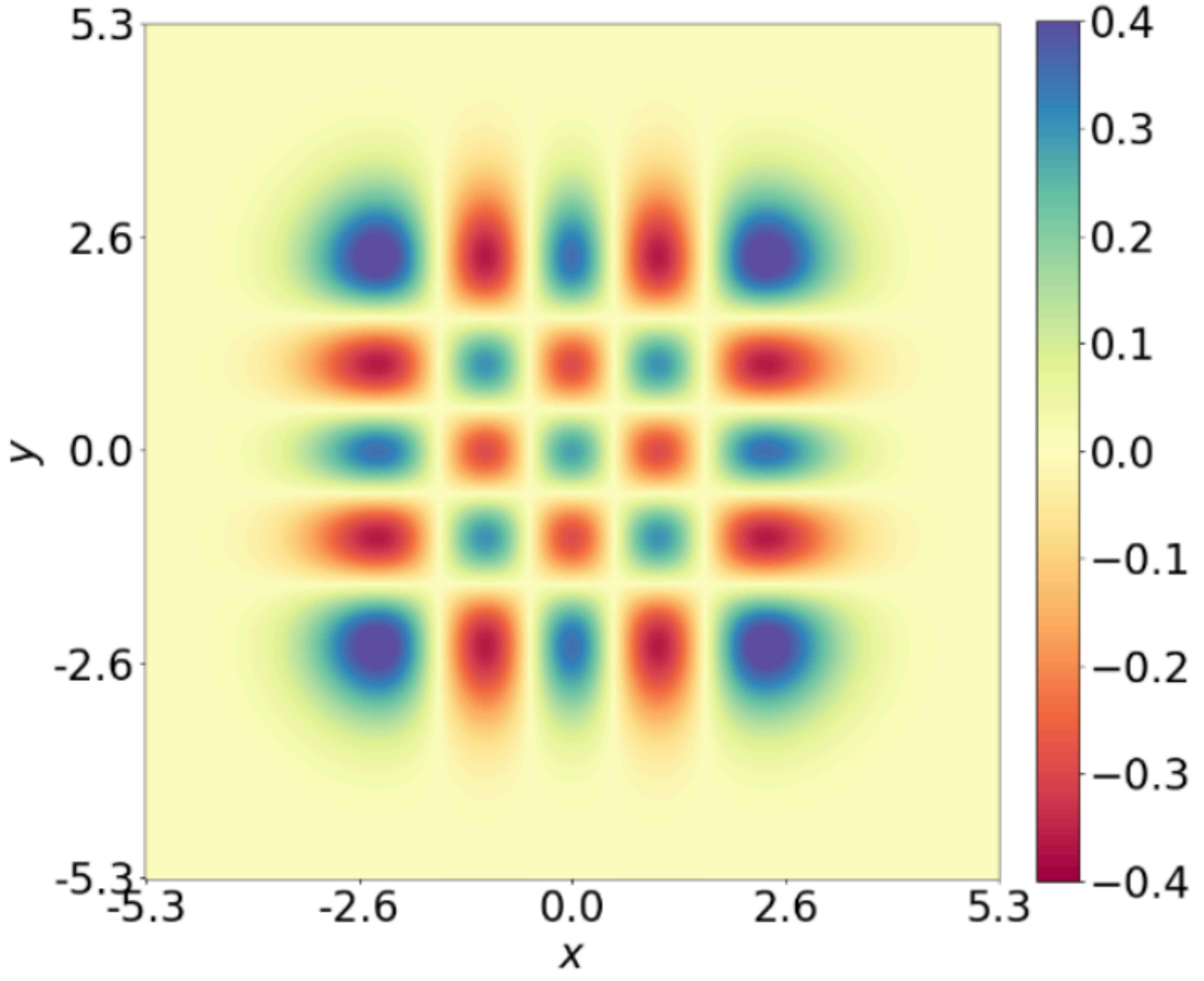


Figure 5: Solution for 2D QHO with $\mu_{gt} = 5$ on $\Omega' = 5.3\Omega$.

	Approximation error		Runtime (s)
	ϵ_μ	ϵ_1	
PINN	6.01	$7.32 \cdot 10^{-2}$	$t \approx 1414$
ID-PINN	$6.21 \cdot 10^{-2}$	$7.51 \cdot 10^{-3}$	$t \approx 1346$
SC-PINN	$2.18 \cdot 10^{-4}$	$5.68 \cdot 10^{-4}$	$t \approx 192$
GF-PSM	$\mathbf{1.50 \cdot 10^{-10}}$	$\mathbf{5.13 \cdot 10^{-9}}$	$t \approx \mathbf{5}$

Table 4: Errors for 2D QHO inverse problem with $\mu_{gt} = 5$

Non-Linear Navier Stokes Problems

We consider the incompressible 2D Navier Stokes equation as an example of a non-linear PDE problem: Let $u = (u_1, u_2)$, $u \in C^2(\Omega, \mathbb{R}^2)$ be the vector velocity field and $p \in C^1(\Omega; \mathbb{R})$ the scalar pressure field the equation becomes:

$$\begin{cases} -\nu \Delta u(x,y) + (u(x,y) \cdot \nabla) u(x,y) + \nabla p(x,y) &= f(x,y) \quad ,\forall (x,y) \in \Omega \\ \nabla \cdot u(x,y) &= 0 \quad ,\forall (x,y) \in \Omega \\ u(x,y) - g(x,y) &= 0 \quad ,\forall (x,y) \in \partial\Omega \,, \end{cases}$$

where

$$f(x,y) = 2\nu\pi^2 (u_1(x,y), u_2(x,y)) + \pi \cos(\pi x) \cos(\pi y)(-u_1(x,y), u_2(x,y))$$
$$+ \pi \sin(\pi x) \sin(\pi y)(u_2, -u_1) + \exp(\pi y)(1, \pi x) \,,$$

$$g(x,y) = [-\sin(\pi x)\cos(\pi y), \cos(\pi x)\sin(\pi y)]^T$$

Non-Linear Navier Stokes Problems

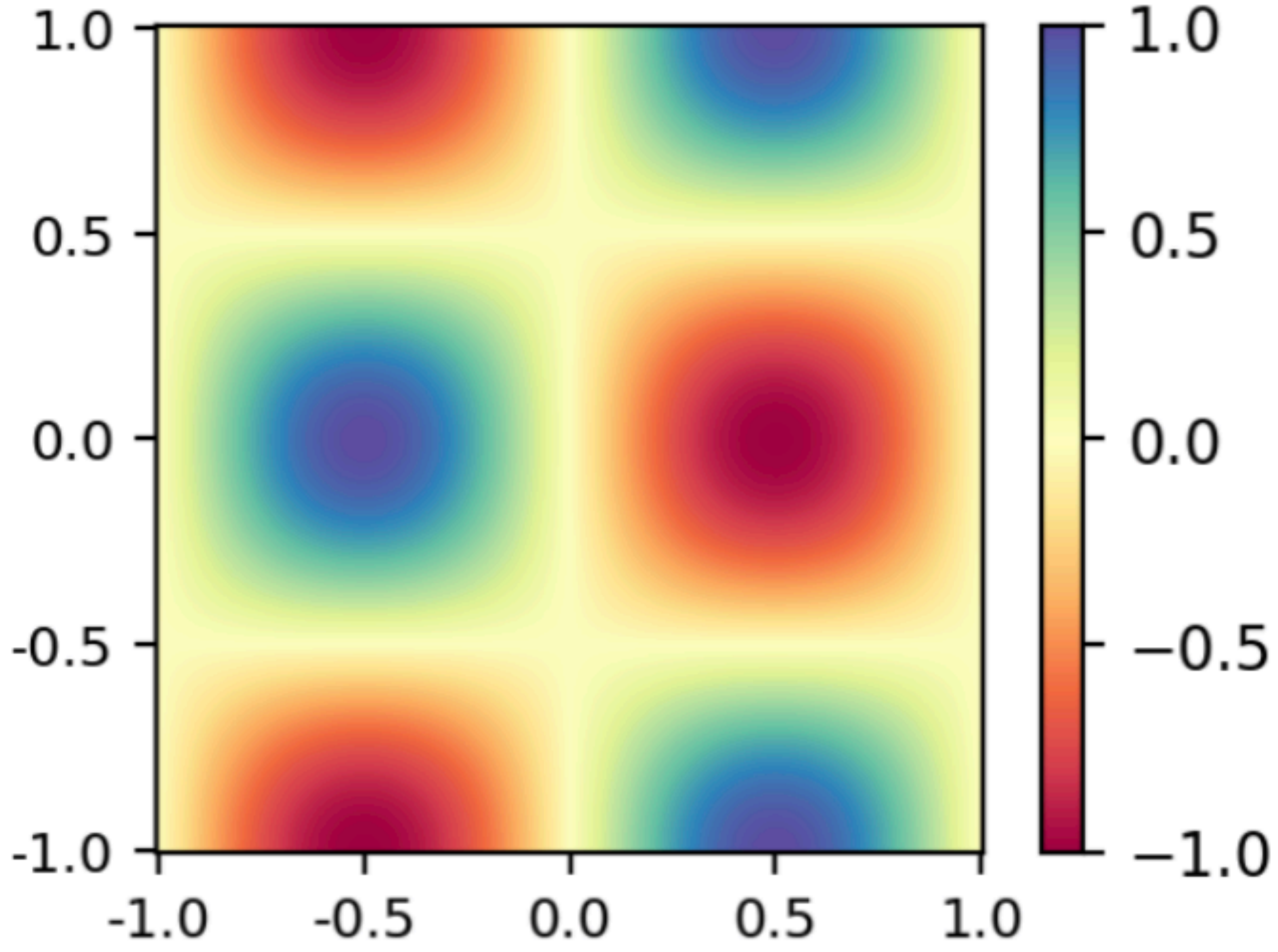


Figure 6: Solution u_1.

	Approximation error		Runtime (s)
Forward Problem	ϵ_1	ϵ_∞	
GF-PSM u_1	$3.31 \cdot 10^{-10}$	$2.35 \cdot 10^{-9}$	$t \approx 405.22$
GF-PSM u_2	$3.28 \cdot 10^{-10}$	$2.35 \cdot 10^{-9}$	$t \approx 405.22$
Inverse Problem	ϵ_ν	ϵ_1	
GF-PSM	$8.9 \cdot 10^{-14}$	$1.07 \cdot 10^{-8}$	$t \approx 395.49$
AD-PSM	$\mathbf{5.9 \cdot 10^{-16}}$	$\mathbf{7.31 \cdot 10^{-15}}$	$t \approx \mathbf{1.75}$

Table 5: Approximation errors

Inverse Problem asks for inferring the viscosity ν and the pressure field !