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Parameterized Physics-informed Neural Networks for Parameterized PDEs

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Introduction

PINNs suffer from **several obvious weaknesses**.

- W1) PDE operators are highly nonlinear (making training extremely difficult);
- W2) Repetitive trainings from scratch are needed when solutions to new PDEs are sought (even for new PDEs arising from new PDE parameters in parameterized PDEs).

There have been various efforts to mitigate each of these issues: (**For addressing W1**) curriculum-learning-type training algorithms that train PINNs from easy PDEs to hard PDEs (Krishnapriyan et al., 2021), and (**for addressing W2**) meta-learning PINNs (Liu et al., 2022); or directly learning solutions of parameterized PDEs such that $u_{\Theta}(x, t; \mu)$, where μ is a set of PDE parameters, e.g., $\mu=[\beta , \nu, \rho]$ in convection-diffusion-reaction (CDR) equations. However, there has been a less focus on addressing both problems in a unified PINN framework.

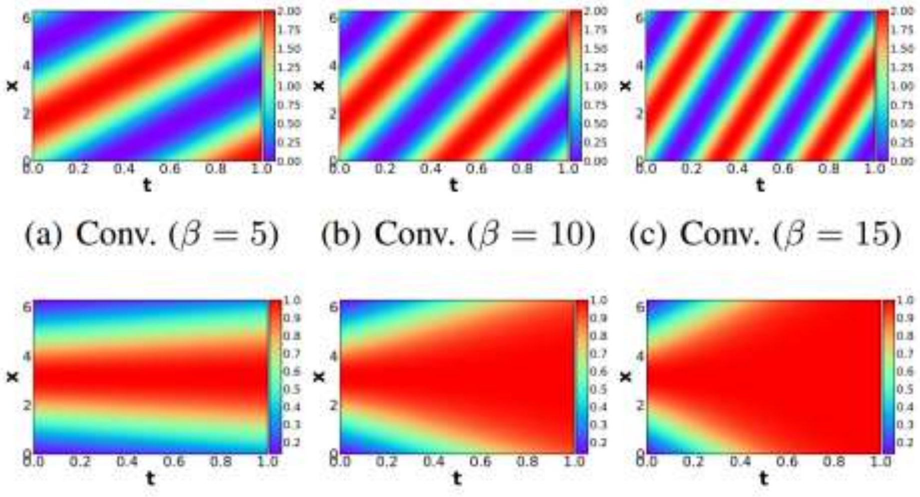
To mitigate the both issues in W1 and W2 simultaneously, we propose a variant of PINNs for solving parameterized PDEs, called parameterized physics-informed neural networks (**P^{2}INNs**). A novel modification proposed in our model is to explicitly extract a hidden representation of the PDE parameters by employing a separate encoder network, $h_{param} = g_{\Theta_p}(\mu)$, and uses this hidden representation to parameterize the solution neural network, $u_{\Theta}(x, t; h_{param})$.

Motivation

As an example, we consider parameterized CDR equations:

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} - \rho u(1-u) = 0, \quad x \in \Omega, \quad t \in [0, T].$$

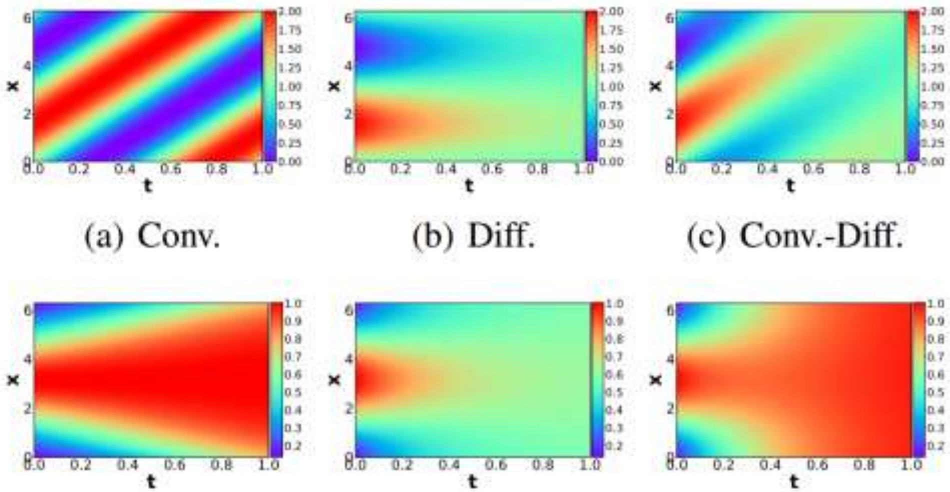
convective diffusive reactive



(a) Conv. ($\beta = 5$) (b) Conv. ($\beta = 10$) (c) Conv. ($\beta = 15$)

(d) Reac. ($\rho = 1$) (e) Reac. ($\rho = 4$) (f) Reac. ($\rho = 7$)

Figure 2. The ground-truth solutions of various convection equations with an initial condition of $1 + \sin(x)$ (Figure 2. (a)-(c)) and reaction equations with an initial condition of a Gaussian distribution $N(\pi, (\pi/2)^2)$ (Figure 2. (d)-(f)). We note that varied solutions are made (with similar architectures) depending on changes in coefficient.



(a) Conv. (b) Diff. (c) Conv.-Diff.

(d) Reac. (e) Diff. (f) Reac.-Diff.

Figure 3. The ground-truth solutions of various CDR equations with an initial condition of $1 + \sin(x)$ (Figure 3. (a)-(c)) or a Gaussian distribution $N(\pi, (\pi/2)^2)$ (Figure 3. (d)-(f)). We note that the solution in the last column reflects the first two columns' solutions. Therefore, there also exist similarities across different equation types.

参数化PDE的解可能存在一个共同的潜在空间

P^2INNs : Parameterized PINNs

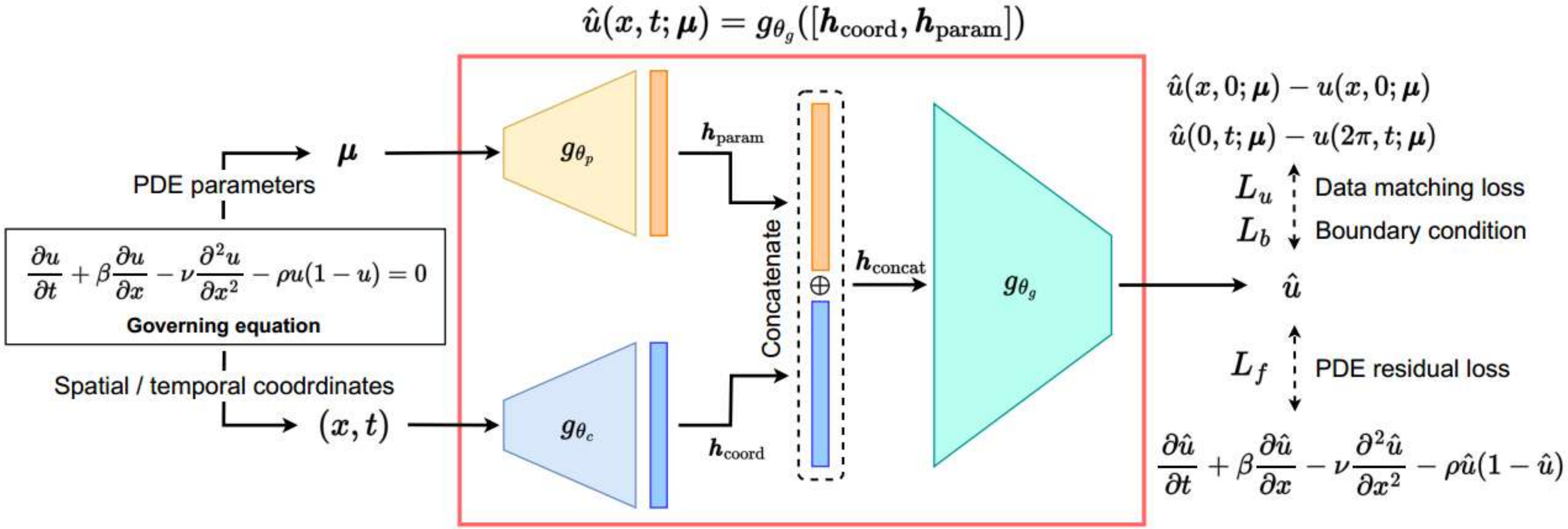


Figure 4. **P^2INNs architecture.** The two encoders g_{θ_p} and g_{θ_c} are added to generate better representations for the PDE parameter and the spatial/temporal coordinate. We also customize the manifold network g_{θ_g}. In this figure, we provide the CDR equation as an example.

encoder for equation input: $\boldsymbol{h}_{\text{param}} = \sigma(FC_{D_p} \cdots (\sigma(FC_2(\sigma(FC_1(\boldsymbol{\mu})))))), \quad (3)$

encoder for spatiotemporal coordinate: $\boldsymbol{h}_{\text{coord}} = \sigma(FC_{D_c} \cdots (\sigma(FC_2(\sigma(FC_1(x,t)))))), \quad (4)$

manifold network: $\hat{u}(x,t;\boldsymbol{\mu}) = \sigma(FC_{D_g} \cdots \sigma(FC_1(\boldsymbol{h}_{\text{concat}}))), \quad (5)$

Where $\boldsymbol{h}_{\text{concat}} = \boldsymbol{h}_{\text{coord}} \oplus \boldsymbol{h}_{\text{param}}$, and $\oplus$ is the concatenation of the two vectors

Train

our basic loss function consists of three terms as follows:

$$L(\Theta) = w_1 L_u + w_2 L_f + w_3 L_b, , \qquad (6)$$

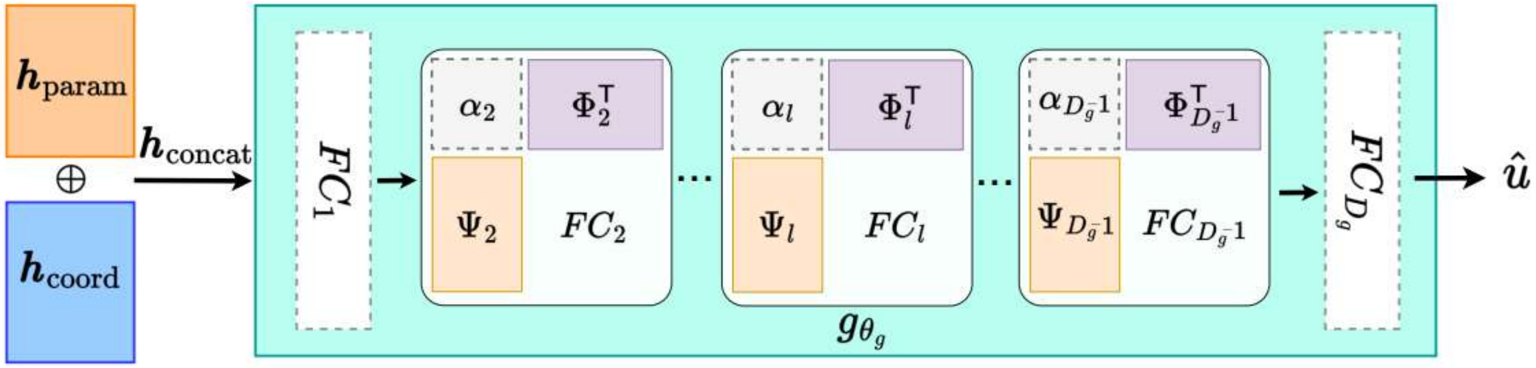
where L_u, L_b and L_f enforces initial, boundary conditions, and physical laws in PDEs, respectively, and $\omega_1, \omega_2, \omega_3$ are hyperparameters. In general, the overall training method follows the training procedure of the original PINN.

$$L_u = \frac{1}{N_u} \sum_{N_u} \Big(\hat{u}(x, 0; \boldsymbol{\mu}) - u(x, 0; \boldsymbol{\mu}) \Big)^2,$$

$$L_f = \frac{1}{N_f} \sum_{N_f} \Big(\mathcal{F}(x, t, \hat{u}; \boldsymbol{\mu}) \Big)^2,$$

$$L_b = \frac{1}{N_b} \sum_{N_b} \Big(\hat{u}(0, t; \boldsymbol{\mu}) - \hat{u}(2\pi, t; \boldsymbol{\mu}) \Big)^2,$$

SVD微调



each layer, excluding the first and last layers,is decomposed as follows:

$$FC_l = \Psi_l \alpha_l \Phi_l^\top, \quad l = 2, 3, \ldots, D_g - 1. \qquad (7)$$

P^{2}INNs with SVD modulation. From the pre-trained decoder layer of **P^{2}INNs** , we obtain the bases $\Phi_l, \Psi_l$for parameterized PDEs through SVD . Note that only the diagonal matrices α_l are used for fine-tuning. (The dotted lines represent learnable parameters.)

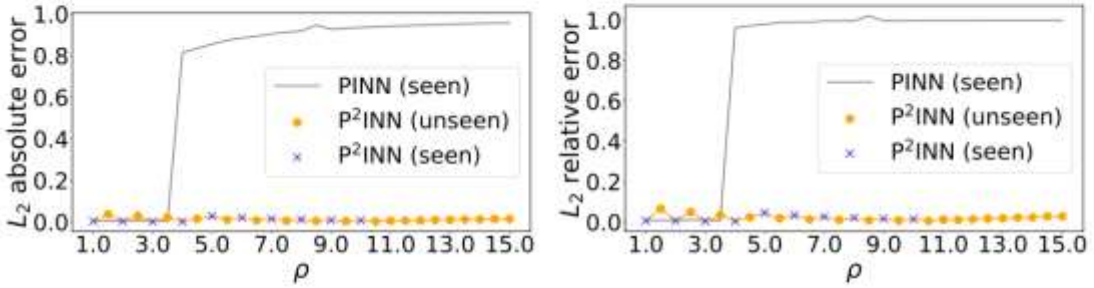
Evaluation

Table 2. The relative and absolute L_2 errors over all the equations. Our P^2INNs surpass baselines in all but one cases, even without fine-tuning. IMP. denotes the rate of improvement of our model over the best baseline.

	PDE type	Coefficient range	Metric	PINN	PINN-R	PINN-seq2seq	P^2INN	IMP. (%)
Class 1	Convection	1~5	Abs. err.	0.0183	0.0222	0.1281	**0.0039**	78.44
			Rel. err.	0.0327	0.0381	0.2160	**0.0079**	75.82
		1~10	Abs. err.	0.0164	0.0666	0.1924	**0.0093**	43.62
			Rel. err.	0.0307	0.1195	0.3276	**0.0179**	41.78
		1~20	Abs. err.	0.1140	0.1624	0.2252	**0.0198**	82.64
			Rel. err.	0.1978	0.2779	0.3819	**0.0464**	76.55
	Diffusion	1~5	Abs. err.	0.1335	0.1665	0.1987	**0.1322**	0.97
			Rel. err.	0.2733	0.3462	0.4050	**0.2710**	0.84
		1~10	Abs. err.	0.2716	0.3175	0.3149	**0.1539**	43.34
			Rel. err.	0.5259	0.6206	0.6174	**0.3116**	40.75
		1~20	Abs. err.	0.6782	0.7054	0.3346	**0.1916**	42.74
			Rel. err.	1.2825	1.3401	0.6442	**0.3745**	41.87
	Reaction	1~5	Abs. err.	0.3341	0.3336	0.4714	**0.0015**	99.54
			Rel. err.	0.3907	0.3907	0.5907	**0.0027**	99.31
		1~10	Abs. err.	0.6232	0.3619	0.6924	**0.0065**	98.19
			Rel. err.	0.6926	0.4190	0.7931	**0.0089**	97.88
		1~20	Abs. err.	0.7902	0.4320	0.8246	**0.0042**	99.02
			Rel. err.	0.8460	0.4932	0.8960	**0.0092**	98.14
Class 2	Conv.-Diff.	1~5	Abs. err.	0.0610	0.0654	0.0979	**0.0399**	34.61
			Rel. err.	0.1175	0.1289	0.1950	**0.0892**	24.05
		1~10	Abs. err.	0.1133	0.1313	0.0917	**0.0576**	37.25
			Rel. err.	0.2098	0.2510	0.1959	**0.1320**	32.62
		1~20	Abs. err.	0.2735	0.2118	0.0645	**0.0622**	3.51
			Rel. err.	0.5106	0.4154	0.1504	**0.1485**	1.28
	Reac.-Diff.	1~5	Abs. err.	0.1900	0.1876	0.4201	**0.1225**	34.70
			Rel. err.	0.2702	0.2777	0.5346	**0.1856**	31.31
		1~10	Abs. err.	0.5166	0.3809	0.6288	**0.1833**	51.88
			Rel. err.	0.6141	0.4790	0.7274	**0.2756**	42.46
		1~20	Abs. err.	0.7167	0.7210	0.7663	**0.0898**	81.03
			Rel. err.	0.7998	0.8105	0.8337	**0.1411**	74.68
Class 3	Conv.-Diff.-Reac.	1~5	Abs. err.	0.1663	0.0865	0.4943	**0.0311**	64.02
			Rel. err.	0.2057	0.1415	0.6104	**0.0525**	62.88
		1~10	Abs. err.	0.5321	0.3170	0.7051	**0.0508**	83.98
			Rel. err.	0.5928	0.3772	0.8027	**0.0939**	75.10
		1~20	Abs. err.	0.7450	0.4080	0.7136	**0.0353**	91.94
			Rel. err.	0.7960	0.4645	0.8100	**0.0812**	82.88

1D CDR Equations

Evaluation

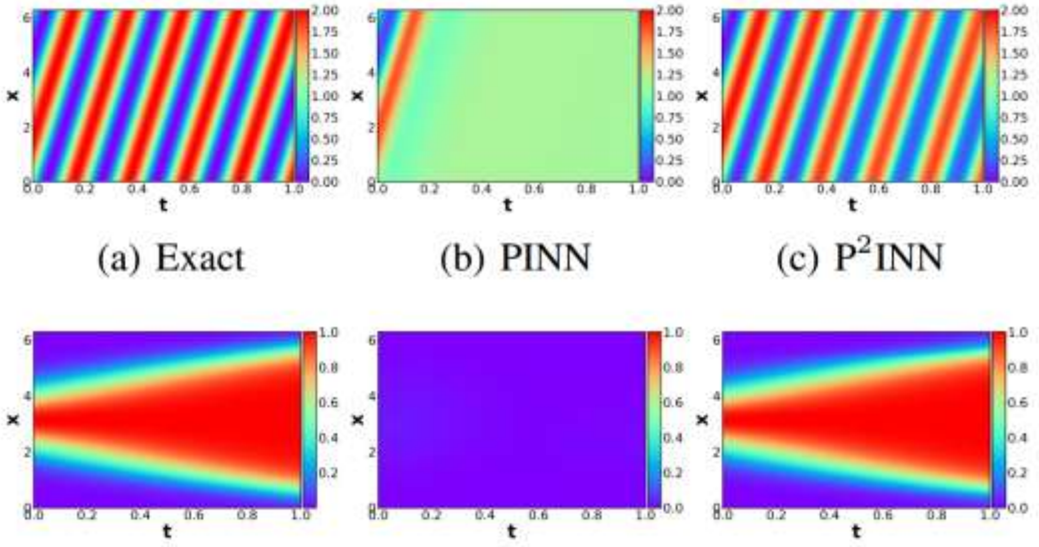


(a) L_2 absolute error (b) L_2 relative error

Figure 6. [Reaction equation] Interpolation and extrapolation results for unseen ρ.

Table 4. Experimental results of modulations with an initial condition of a Gaussian distribution $N(\pi, (\pi/2)^2)$.

PDE type	Metric	PINN (best)	P^2INN	Modulation All	Modulation Shift	Modulation SVD
Convection	Abs. err.	0.0183	0.0174	0.1959	0.0139	**0.0138**
	Rel. err.	0.0327	0.0316	0.3319	0.0248	**0.0246**
Reaction	Abs. err.	0.3336	0.0126	0.0713	0.0095	**0.0089**
	Rel. err.	0.3907	0.0229	0.1211	0.0198	**0.0184**
Conv.-Diff.-Reac.	Abs. err.	0.0865	0.0315	0.0463	0.0321	**0.0303**
	Rel. err.	0.1415	0.0508	0.0690	0.0521	**0.0486**



(a) Exact (b) PINN (c) P^2INN

(d) Exact (e) PINN (f) P^2INN

Figure 7. Failure modes in the convection equation of $\beta = 30$ (a-c), and the reaction equation of $\rho = 5$ (d-f). P^2INNs much more accurately predict reference solutions.

Table 3. Ablation study on the reaction equations.

Coefficient range	PINN-P Abs. err.	PINN-P Rel. err.	P^2INN Abs. err.	P^2INN Rel. err.
1∼5	0.0083	0.0113	0.0015	0.0027
1∼20	0.8975	0.9908	0.0042	0.0092

Thanks!