Predicting the stabilization quantity with neural networks for Singularly Perturbed Partial Differential Equations

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Convection Diffusion Equation

$$\underbrace{-\epsilon\Delta u}_{\text{Diffusion term}} + \underbrace{\mathbf{b}.\nabla u}_{\text{Convection term}} = \underbrace{f}_{\text{Source term}} \quad \text{in } \Omega$$

$$u = u_b \text{ on } \Gamma^D,$$

Variable	Description	Variable	Description
$\Omega \subset \mathbb{R}^n$	Bounded Domain	$x \in \Omega \cup \Gamma$	Spatial point in Domain
ϵ	Diffusion coefficient	$u(x)$	Unknown scalar function
$\mathbf{b} \in W^{1,\infty}(\Omega)^2$	Convective velocity	$u_b \in H^{1/2}(\Gamma^D)$	Dirichlet boundary value
$f \in L^2(\Omega)$	External source term		

Singularly Perturbed Differential Equations (SPDE)

$$-\epsilon u''(x) + u'(x) = 1, \text{ for } x \in (0,1),$$
$$u(0) = u(1) = 0$$

Suppose, we set $\epsilon = 0$, the above example will be converted as first-order ODE

$$u'(x) = 1 \text{ for } 0 < x < 1$$

- The exact solution will not satisfy both boundary conditions
- This problem has no solution in $C^1[0,1]$
- We infer that when ϵ is near zero, the solution behaves badly in some way
- These types of differential equations are called singularly perturbed differential equations (SPDE)

Singularly Perturbed Differential Equations (SPDE)

- Solution approaches a discontinuous limit when $\epsilon \to 0$ and $x = 1$
- Due to this boundary layer, the numerical solution shows spurious oscillations.
- Stabilization techniques are used to get rid of these spurious oscillations
- Finding an optimal stabilization parameter is a challenge

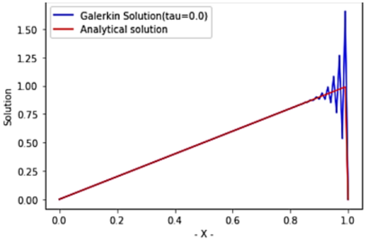


Figure: Oscillations in Galerkin solution

Numerical Schemes for Partial Differential Equation

Conventional Numerical techniques

- Finite Difference Method
- Finite Element Method
- Finite Volume Method

Stabilization Techniques

- Local Projection Stabilization
- Streamline Upwind Petrov Galerkin (SUPG)

Neural Network-based PDE solvers

- Physics Informed Neural Network
- DeepONet
- Fourier Neural Operator

Galerkin Weak Form of the SPDE

Find u such that for all $v \in H_0^1(\Omega)$

$$a(u, v) = (f, v) \tag{1}$$

where the bilinear form $a(\cdot, \cdot) : H^1(\Omega) \times H_0^1(\Omega) \to R$ is defined by

$$a(u, v) = \int_\Omega \epsilon u' v' dx + \int_\Omega b u' v dx \tag{2}$$

$$(f, v) = \int_\Omega f v dx \tag{3}$$

$(\cdot, \cdot)$ is the $L^2(\Omega)$ inner product.

Streamline Upwind Petrov Galerkin Technique(SUPG)

The residual of equation is :

$$R(u) = -\epsilon u'' + bu' - f \tag{4}$$

Modified weak form: Find $u_h \in V_h$ such that:

$$\begin{aligned} a_h(u_h, v_h) &= \epsilon(\nabla u_h, \nabla v_h) + (\mathbf{b} \cdot \nabla u_h, v_h) \\ &+ \sum_{i \in \Omega_h} \underbrace{\tau_i(-\epsilon \Delta u_h + \mathbf{b} \cdot \nabla u_h - f_h, \mathbf{b} \cdot \nabla v_h)_{\Omega_h}}_{\text{Stabilization term}} \\ &= (f, v_h) + (g, v_h)_{\Gamma^N} \quad \forall v_h \in V_h \end{aligned} \tag{5}$$

$\tau_i \in L^2(\Omega)$ is a user-chosen stabilization parameter.

Stabilization Parameter τ

Standard formula:

$$\text{For local Peclet number, } Pe = \frac{bh}{2\epsilon};$$
$$\tau = \frac{h}{2b}(\coth(Pe) - \frac{1}{Pe}); \tag{6}$$
$$\text{where } coth = \frac{\exp(x) + \exp(-x)}{\exp(x) - \exp(-x)}$$

Limitations:

- Std. τ gives the exact solution only for the 1D problems
- Std. τ technique has limited performance in complex cases

Objective: Develop a Neural Network model to identify an optimal stabilization parameter for 1D and 2D cases

SPDE-Net

- Developed an ANN-based supervised and L^2 EM techniques for predicting the stabilization parameter in the SUPG method for one-dimensional SPDEs.
- Developed a training dataset based on the equation coefficients and demonstrated the prediction of global and local variants of stabilization parameter τ with ANN.
- Showed that ANN-aided FEM solvers solve one-dimensional SPDEs with lesser numerical error than that with pure neural network solvers such as PINNs.

[4]Sangeeta Yadav, Sashikumaar Ganesan, “SPDE-Net: Neural Network based prediction of stabilization parameter for SUPG technique”, Proceedings of the 13th Asian Conference on Machine Learning, PMLR 157:268-283, 2021

SPDE-Net for 1D convection-diffusion equation

$$\hat{\tau}_i(\theta) = G_\theta(\epsilon_i, b_i, h_i) \tag{7}$$

$$\hat{u}_i(\theta) = H(\epsilon_i, b_i, h_i, \hat{\tau}_i) \tag{8}$$

$$\theta^*_{supervised} = argmin \sum_{i=1}^{N} loss\left(\hat{\tau}_i(\theta), \tau_i\right) \tag{9}$$

$$\theta^*_{L^2 \text{ Error Minimization}} = argmin \sum_{i=1}^{N} loss\left(\hat{u}_i(\theta), u_i\right) \tag{10}$$

where, G_θ is θ parameterized SPDE-Net, H is the FEM solution, τ_i is the stabilization parameter, u is the analytical solution and N is the number of training examples.

SPDE-Net

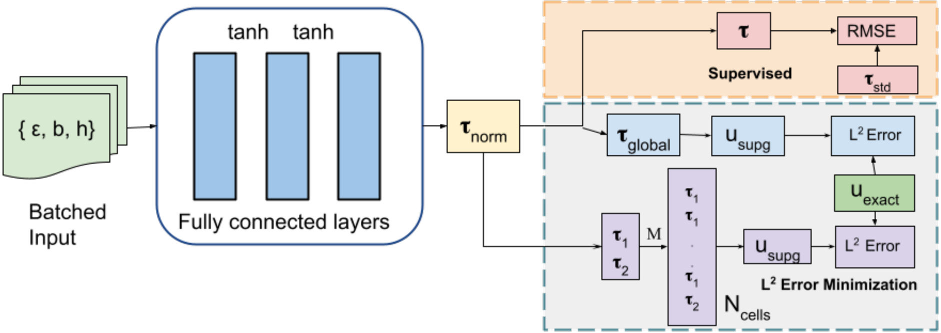


Figure: *SPDE-Net*: An end-to-end deep learning+FEM framework for solving SPDE

L^2 Error Minimization

- Global $\hat{\tau}$: Predict single τ for whole domain.
- Local $\hat{\tau}$: Predict 2 values, $\hat{\tau}_1$ and $\hat{\tau}_2$ for non-boundary and boundary layer regions. In this particular case, the boundary region is either near $x = 0$(for $b < 0$) or $x = 1$(for $b > 0$). For $b > 0$:

$$M = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ \vdots & \vdots \\ 0 & 1 \end{bmatrix}_{N_{\text{cells}},2} \tag{11}$$

$$\tau_{pred} = [\hat{\tau}_1(\theta), \hat{\tau}_2(\theta)]^T \tag{12}$$

$$\hat{\tau}_{local} = M\tau_{pred} \tag{13}$$

Evaluation Metrics

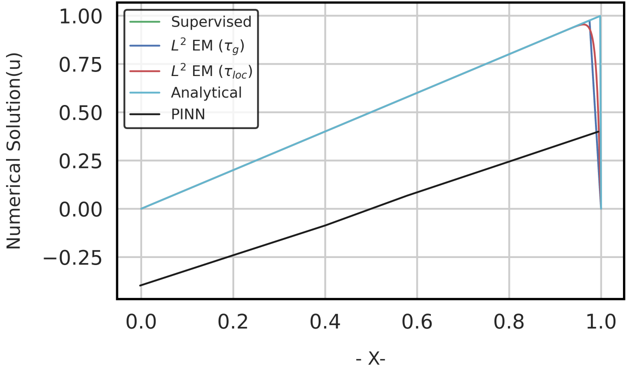
$$RMSE = \frac{\sqrt{\sum_{i=1}^{N} (\hat{\tau} - \tau)^2}}{N} \tag{14}$$

$$L^2 Error = \left(\int_{\Omega} (u_{supg}(\hat{\tau}) - u_{\text{analytical}})^2 dx \right)^{\frac{1}{2}} \tag{15}$$

Qualitative Comparison

Test Case

$\epsilon = 1e - 11, \quad b = 1.0, \quad h = 0.0083$



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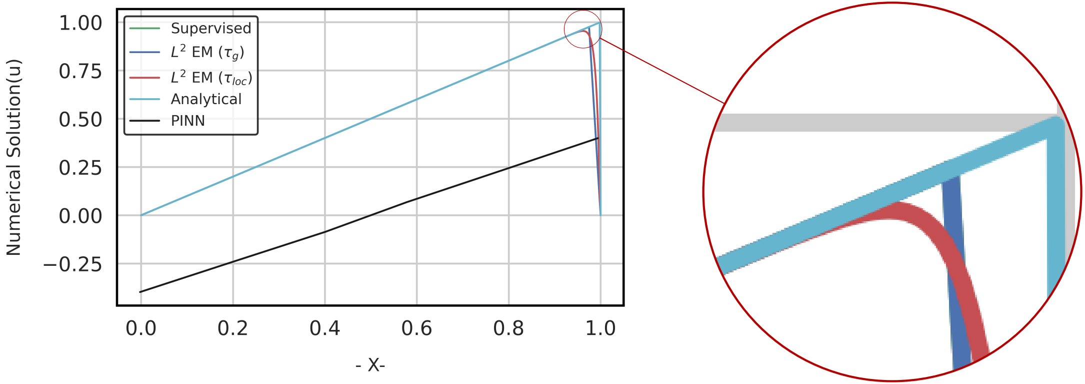

Performance Comparison

Table: Performance comparison of different techniques for validation and test dataset

	Validation data		Test data	
Technique	$\|\|\hat{u}(\hat{\tau}) - u\|\|_{L^2(\Omega_h)}$	$\|\|\hat{\tau} - \tau\|\|_{L^2(\Omega_h)}$	$\|\|\hat{u}(\hat{\tau}) - u\|\|_{L^2(\Omega_h)}$	$\|\|\hat{\tau} - \tau\|\|_{L^2(\Omega_h)}$
PINN	$8.11\,\mathrm{e}{-3}$	NA	$7.82\,\mathrm{e}{-3}$	NA
Supervised	$5.13\,\mathrm{e}{-6}$	$2.79\,\mathrm{e}{-7}$	$7.88\,\mathrm{e}{-6}$	$3.72\,\mathrm{e}{-7}$
L^2 EM(τ_{loc})	$6.42\,\mathrm{e}{-5}$	NA	$1.70\,\mathrm{e}{-4}$	NA
L^2 EM(τ_g)	$\mathbf{5.00}\,\mathrm{e}{-}\mathbf{6}$	$3.33\,\mathrm{e}{-6}$	$\mathbf{7.76}\,\mathrm{e}{-}\mathbf{6}$	$4.83\,\mathrm{e}{-7}$

- SPDE-Net: Neural Network-based prediction of stabilization parameter for SUPG technique Sangeeta Yadav, Sashikumaar Ganesan Proceedings of The 13th Asian Conference on Machine Learning, PMLR 157:268-283, 2021.
- THANK YOU