Change Point - Physics Informed Neural Networks (CP-PINNs)

GitHub: https://github.com/yamansan/CP-PINNs

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Recap

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- Using neural networks, we can also approximate the solutions to partial differential equations.

Goal

- Consider the Advection-Diffusion equation

$$\frac{\partial u(x,t)}{\partial t} + \frac{\partial u(x,t)}{\partial x} = \lambda(t)\frac{\partial^2 u(x,t)}{\partial x^2}$$

with

$$\lambda(t) = \begin{cases} 0.5 & \text{for } t \in [0, \frac{1}{3}), \\ 0.05 & \text{for } t \in [\frac{1}{3}, \frac{2}{3}), \\ 1.0 & \text{for } t \in [\frac{2}{3}, 1). \end{cases}$$

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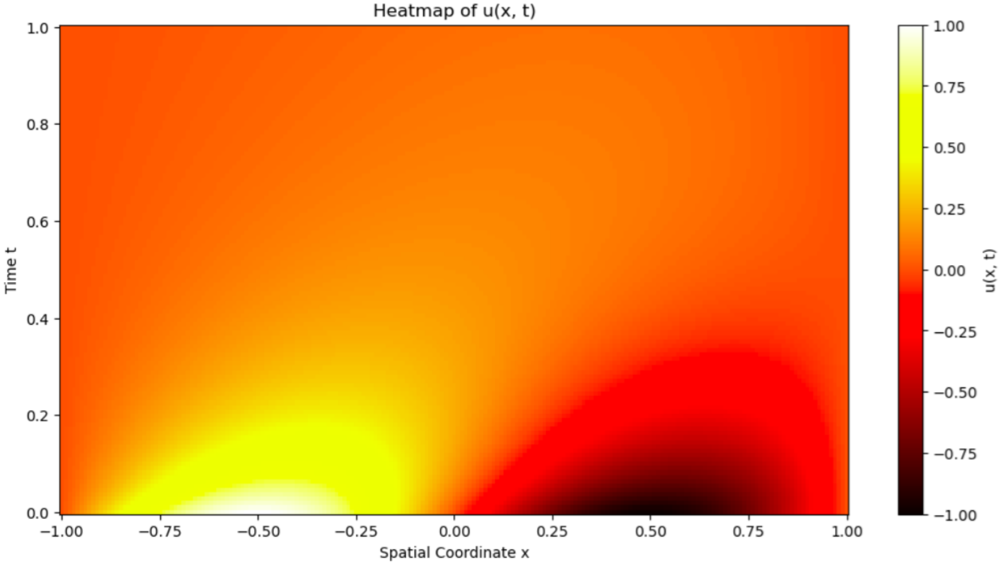
- Given actual data points $u(x,t)$, we want to estimate $\lambda(t)$, hence the change-points too.

Training Data

For training data, we first solve the equation numerically.



Numerical Solution

Figure. Numerical Solution $\frac{\partial u}{\partial x} + \frac{\partial u}{\partial t} = \lambda(t)\frac{\partial^2 u}{\partial x^2}$ with initial conditions $u(x,0) = -sin(\pi x)$ and $u(-1,t) = u(1,t) = 0$

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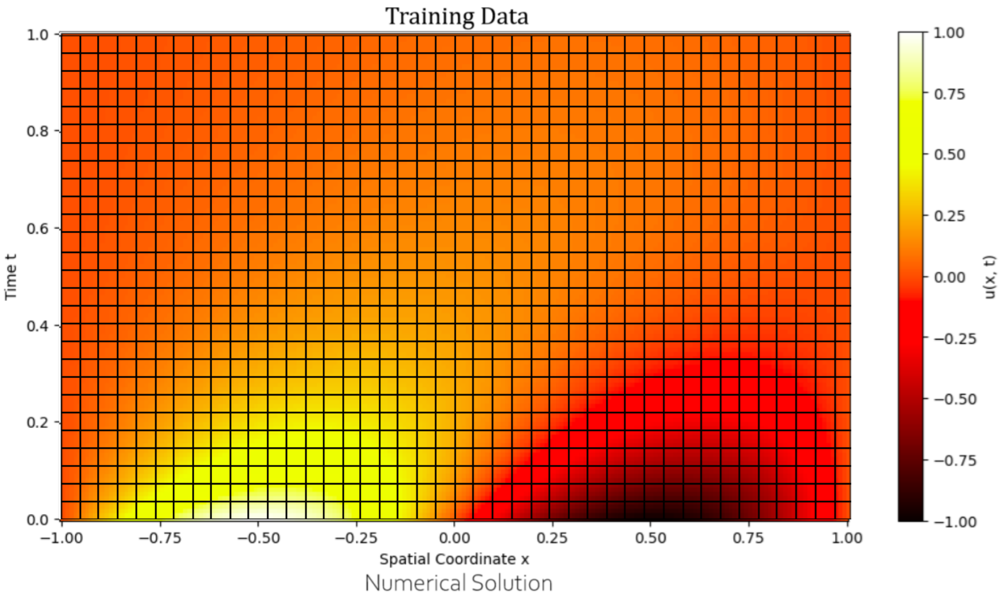
We choose data points from the numerical solution as our training data.



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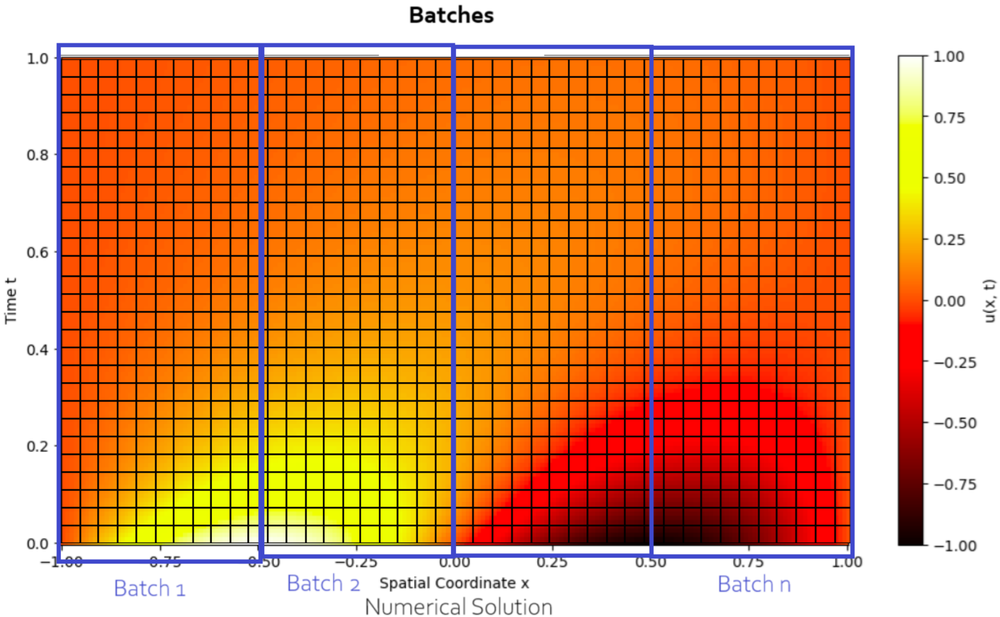

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Loss Function for CP-PINN

- The first loss function term comes from the residual of the PDE

$$L^{NN} = \sum_{i,j} \left(\frac{\partial u_{NN}(x_i, t_j)}{\partial t_j} + \frac{\partial u_{NN}(x_i, t_j)}{\partial x_i} - \lambda_{NN}(t_j) \frac{\partial^2 u_{NN}(x_i, t_j)}{\partial x_i^2} \right)^2$$

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- Third, we define a regularization term for $\lambda(t)$

$$V^{\lambda} = \sum_{i=1}^{T-1} \delta(t^i) \left| \Delta\lambda(t^i) \right|, \tag{1}$$

where $\delta(t)$ is a U-shaped function around $t = 0$.

Training Algorithm for CP-PINNs

- Then we write the total cost function as

$$L(\mathbf{w}; \boldsymbol{\Theta}, \lambda(t)) = w_1 L^{NN} + w_2 L^{Training} + w_3 V^{\lambda} \tag{2}$$

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- For $(k-1)^{th}$ batch, minimize the cost function above w.r.t. the neural network weights $\mathbf{\Theta}$ and then use the to update the weights $\mathbf{w}$ for k^{th} batch

$$\begin{bmatrix} w_1^{(k)} \\ w_2^{(k)} \\ w_3^{(k)} \end{bmatrix} = \begin{bmatrix} \exp\left[-\eta L_{(k-1)}^{NN} - (1-\eta\gamma)\right] \\ \exp\left[-\eta L_{(k-1)}^{Training} - (1-\eta\gamma)\right] \\ \exp\left[-\eta V_{(k-1)}^{\hat{\lambda}} - (1-\eta\gamma)\right] \end{bmatrix}, \tag{3}$$

Using ordinary PINNS for Pre-Training The Model

- To detect change points better, we first train the neural network just over the training data.

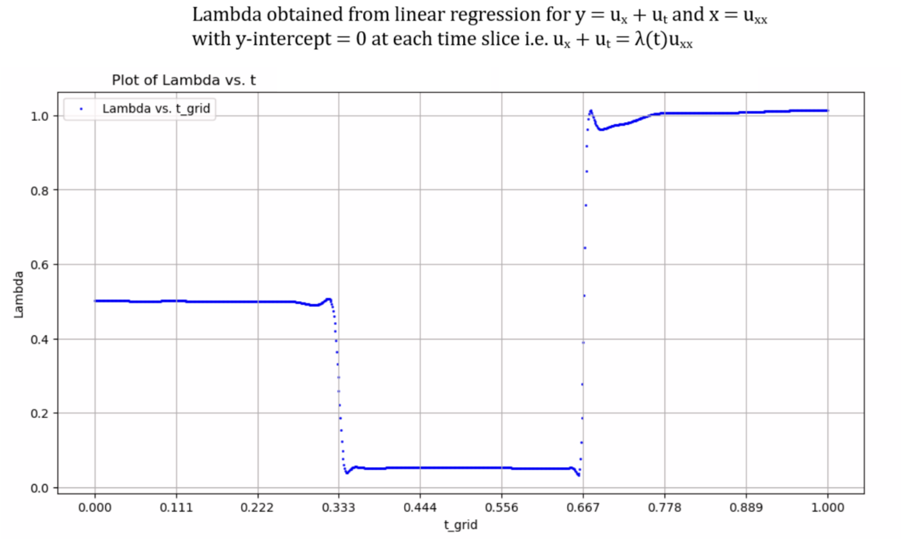

Figure. Lambda obtained from training data without the regularization term V^{λ}

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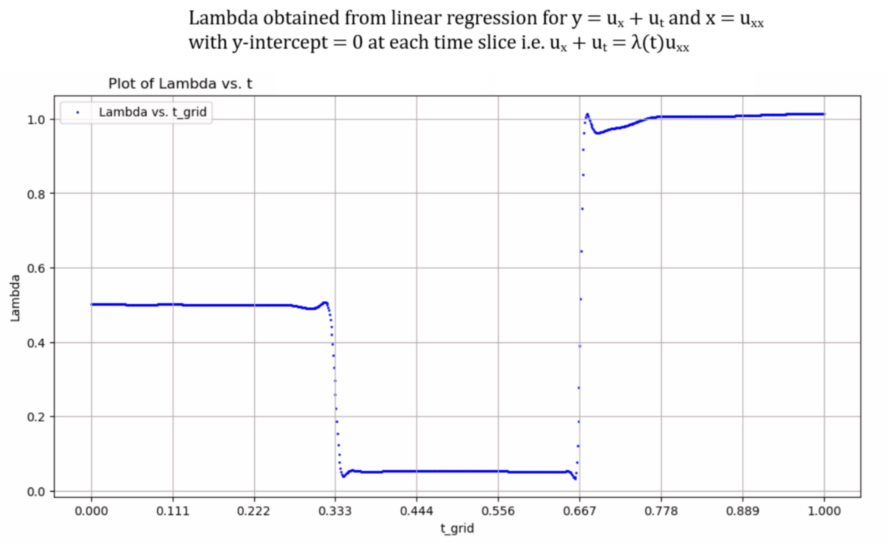
- Let $y = u_x + u_t$ and $x = u_{xx}$ and do a linear regression on $y = \lambda(t)x$ for each t with intercept 0.



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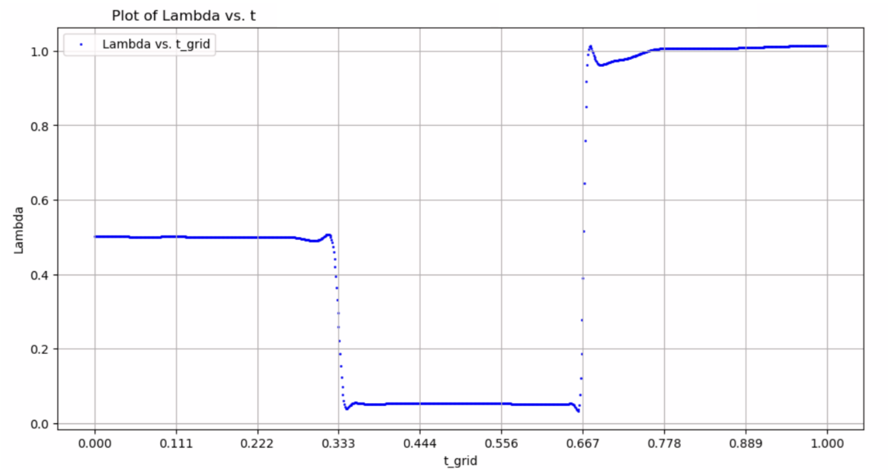
- Let $y = u_x + u_t$ and $x = u_{xx}$ and do a linear regression on $y = \lambda(t)x$ for each t with intercept 0.
- This gives a good estimate of $\lambda(t)$ and the change points.

Lambda obtained from linear regression for $y = u_x + u_t$ and $x = u_{xx}$
with y-intercept = 0 at each time slice i.e. $u_x + u_t = \lambda(t)u_{xx}$



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Training the Model with Pre-Trained Parameters

- Using the pre-trained parameters as initial parameters in our CP-PINN algorithm, we obtain the following $\lambda(t)$

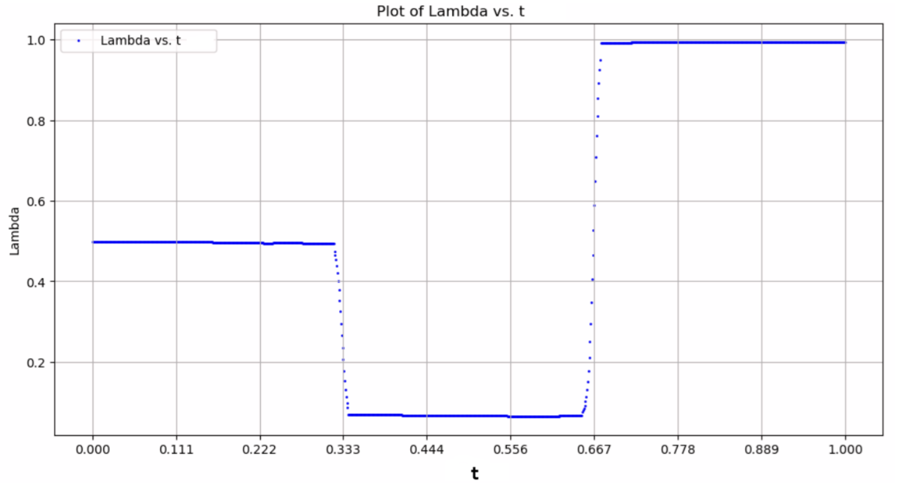
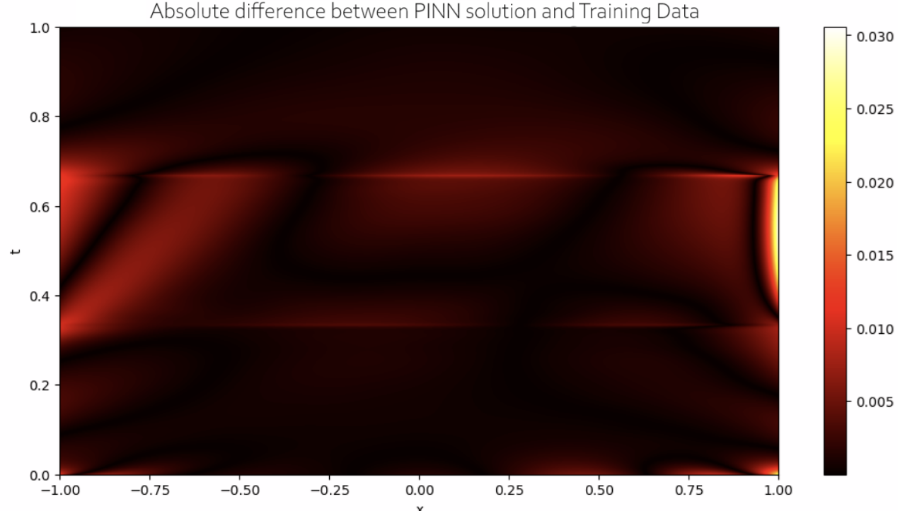


Figure. Lambda obtained from CP-PINN training.

Training The Model with Pre-Trained Parameters

- The absolute error between the training data and the neural network solution



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- Values of $\lambda_1 = 0.5 \pm 0.0017$, $\lambda_2 = 0.05 \pm 0.0011$ and $\lambda_3 = 1.0 \pm 0.0007$

CP-PINNs: Summary and Next Steps

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- Another training algorithm could be to use quadratic programming for optimizing the parameter $\lambda(t)$ for each batch and use Adam for the neural network parameters.
- One may use CP-PINNs in quantitative finance, for instance, to estimate points of high volatility if we think of high-volatility as change points.