Data-Driven Discovery of Partial Differential Equations

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Introduction

Partial differential equations(PDE), commonly regarded as a valuable tool in describing physical and biological studies, are used to mathematically formulate how a system works[1]. Traditionally the governing PDEs are derived analytically, but this has its limitations when it comes to certain complex systems. Data-driven methods allow researchers to discover the governing PDEs based solely on the collected data, which are often measurements taken at different times or positions. This project aims to explore the data-driven method by testing them on three basic types of PDEs: the advection equation, the diffusion equation, and Burger's equation.

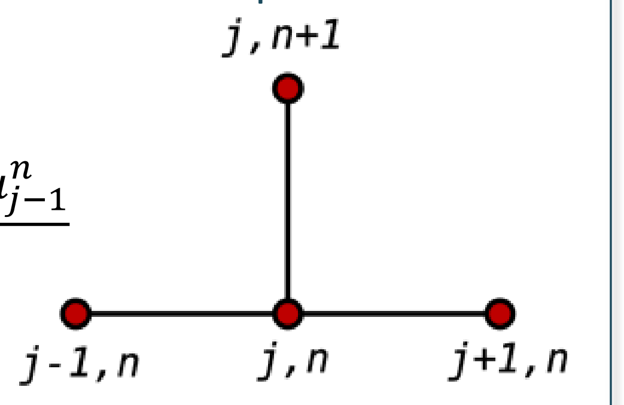
Mathematical Models

The study of each PDE is divided into three steps:

Step 1. Derive numerical solution. Use finite difference methods(FFM) to obtain the numerical solution of the PDE, which gives the data needed for the data-driven method. This project uses two kinds of FFM: Forward difference for time derivative, central difference for space derivative(FTCS) and Crank-Nicholson method.

- FTCS: $u_j^n = u(j\Delta x, n\Delta t)$

$$u_t \approx \frac{u_j^{n+1}-u_j^n}{\Delta t}, u_x \approx \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}, u_{xx} \approx \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}$$

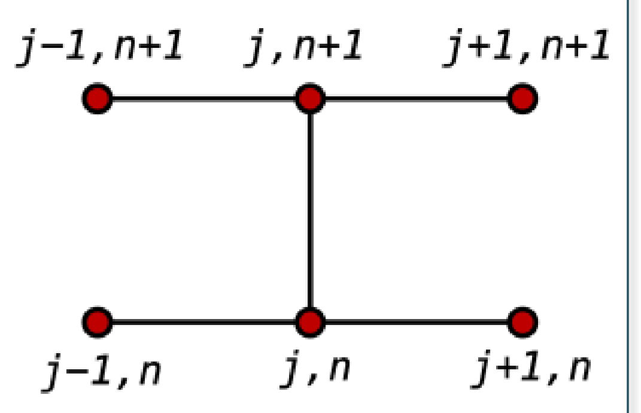


- Crank-Nicholson:

$$u_t \approx \frac{u_j^{n+1}-u_j^n}{\Delta t}$$

$$uu_x \approx \frac{1}{2}\left(u_j^n \frac{u_{j+1}^{n+1}-u_{j-1}^{n+1}}{2\Delta x} + u_j^{n+1}\frac{u_{j+1}^n-u_{j-1}^n}{2\Delta x}\right)$$

$$u_{xx} \approx \frac{1}{2}\left(\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} + \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}\right)$$



Step 2. Apply data-driven method. Feed the data generated in step 1 to PDE-FIND[2], which will return a PDE that has been determined to govern the data.

Step 3. Compare and calculate error. Compare the original PDE with the discovered PDE. Check if the program gives a PDE with the correct terms, and calculate the mean and standard deviation of the parameter errors.

The Advection Equation

The advection equation is a simple representation of how a scalar quantity u (like temperature, concentration, etc.) is transported by a fluid moving with a constant velocity c in a single spatial dimension. x and t denote position and time respectively. The equation is given by

$$u_t + cu_x = 0, \qquad x \in \left[-\frac{L}{2}, \frac{L}{2}\right], t \in [0,T]$$

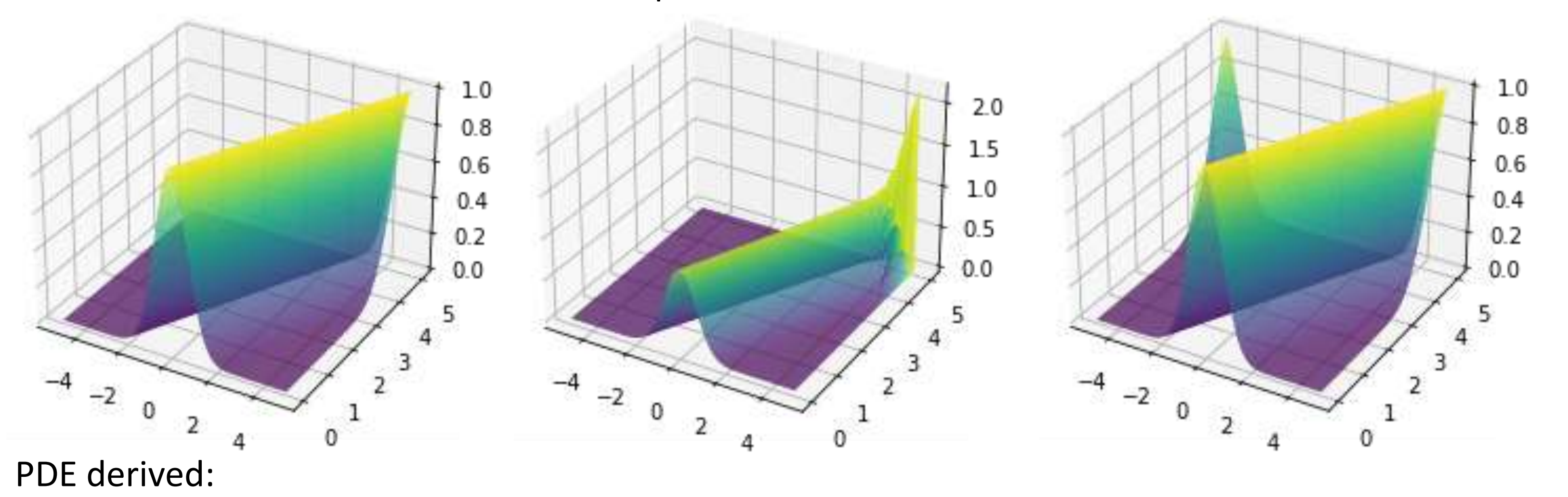
Set Gaussian initial condition and periodic boundary condition:

$$u(x,0) = e^{-x^2}, \qquad u\left(-\frac{L}{2}, t\right) = u\left(\frac{L}{2}, t\right)$$

As the advection equation can be solved analytically, first generate its exact solution, and use FTCS and Crank-Nicholson to obtain numerical solutions. Note that FTCS is unstable in this case and thus errors will accumulate, while Crank-Nicholson is stable.

Set c = 1. Use the generated data as input for PDF-FIND and compare results.

Exact Solution | Explicit Solution | Crank-Nicholson Solution



PDE derived:

$$u_t = -1.004763u_x \qquad u_t = 0.000030uu_{xxx} \qquad u_t = -0.999448u_x$$

With the unstable FTCS scheme, PDE-FIND failed to produce the correct result. With the exact solution and the Crank-Nicholson solution, the discovered PDEs are roughly the same as the original advection equation.

The Diffusion Equation

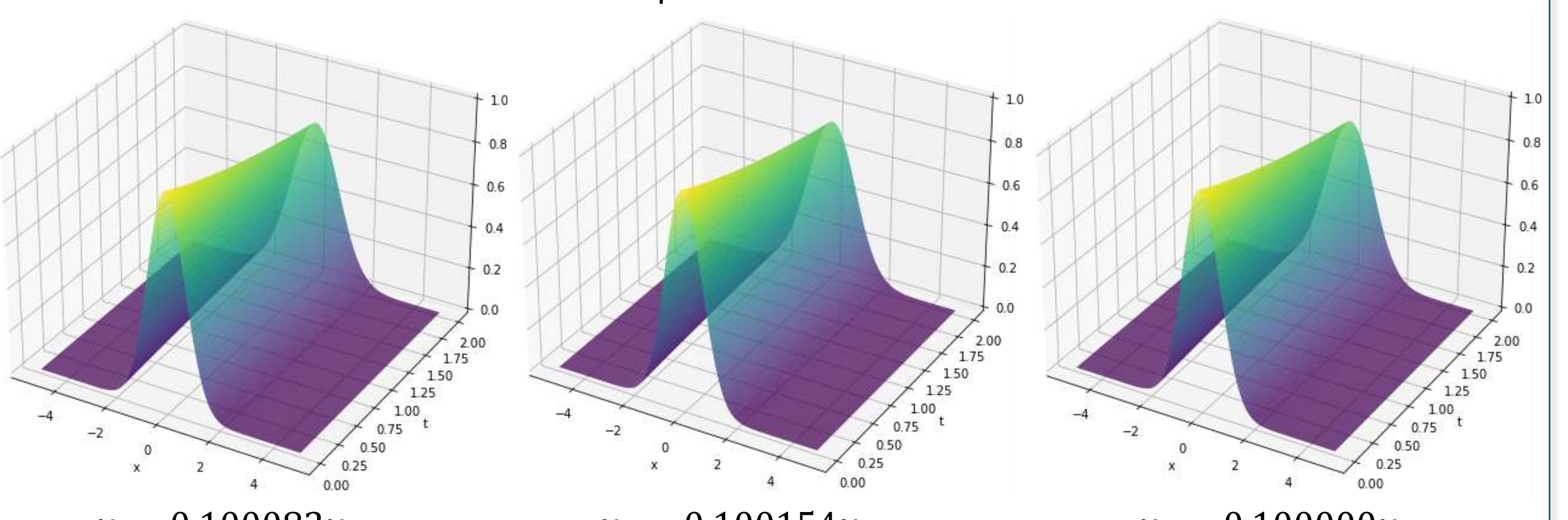
The diffusion equation, also known as the 1D heat equation, describes how heat (or similar diffusive scalar quantity) is distributed over time in a one-dimensional system. The heat equation deals with the spreading or dissipation of heat due to diffusion. The equation is given by

$$u_t = Du_{xx}, \qquad x \in \left[-\frac{L}{2}, \frac{L}{2}\right], t \in [0,T]$$

where u is the concentration or temperature at a given position x and time t, and D is the diffusion coefficient. Set the same Gaussian initial condition and periodic boundary condition.

Set D = 0.1. Here FTCS is stable under certain condition* and Crank-Nicholson is unconditionally stable. Experiments show that for each solution, PDE-FIND gives almost equally accurate results.

Exact Solution | Explicit Solution | Crank-Nicholson Solution



$$u_t = 0.100082u_{xx} \qquad u_t = 0.100154u_{xx} \qquad u_t = 0.100000u_{xx}$$

Burger's Equation

Burgers' equation is a fundamental partial differential equation from the field of fluid mechanics and nonlinear dynamics. It can be considered as a simplified model for studying shock waves, turbulence, and other phenomena in fluids. The equation is given by

$$u_t + uu_x = \nu u_{xx}, \qquad x \in \left[-\frac{L}{2}, \frac{L}{2}\right], t \in [0,T]$$

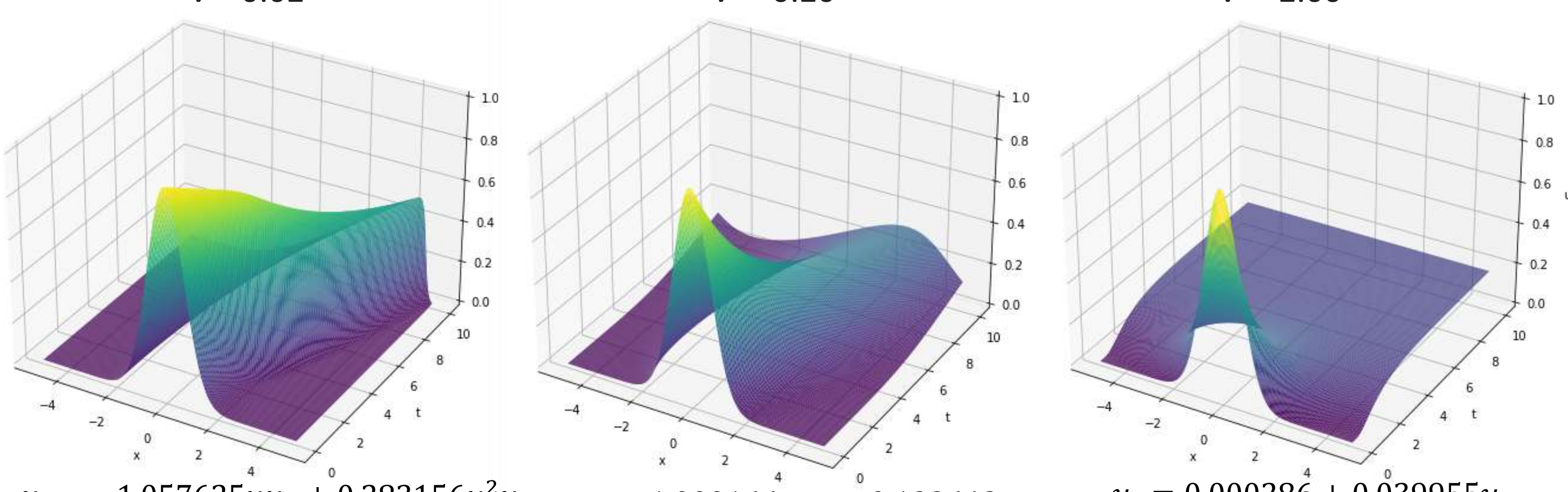
Where u can be thought of as velocity in a fluid flow context, t is time, x is the spatial coordinate, ν is viscosity or diffusion coefficient. Set the same Gaussian initial condition and periodic boundary condition as before.

Unlike the advection equation and the diffusion equation, it is difficult to solve viscous Burger's equation analytically. Apply Crank-Nicholson method to obtain a numerical solution, which has been proved to be consistent and of order two in time and space[3]:

$$\frac{u_j^{n+1}-u_j^n}{\Delta t} + \frac{1}{4\Delta x}\left[u_j^n\left(u_{j+1}^{n+1} - u_{j-1}^{n+1}\right) + u_j^{n+1}\left(u_{j+1}^n - u_{j-1}^n\right)\right] = \frac{\nu}{2(\Delta x)^2}\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1} + u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)$$

The shape of the surface depends largely on the value of ν, and we look at three different values of ν : 0.02, 0.2, 2.0.

ν = 0.02 | ν = 0.20 | ν = 2.00



$$u_t = -1.057625uu_x + 0.283156u^2u_x - 0.258473u^3u_x + 0.019123u_{xx}$$

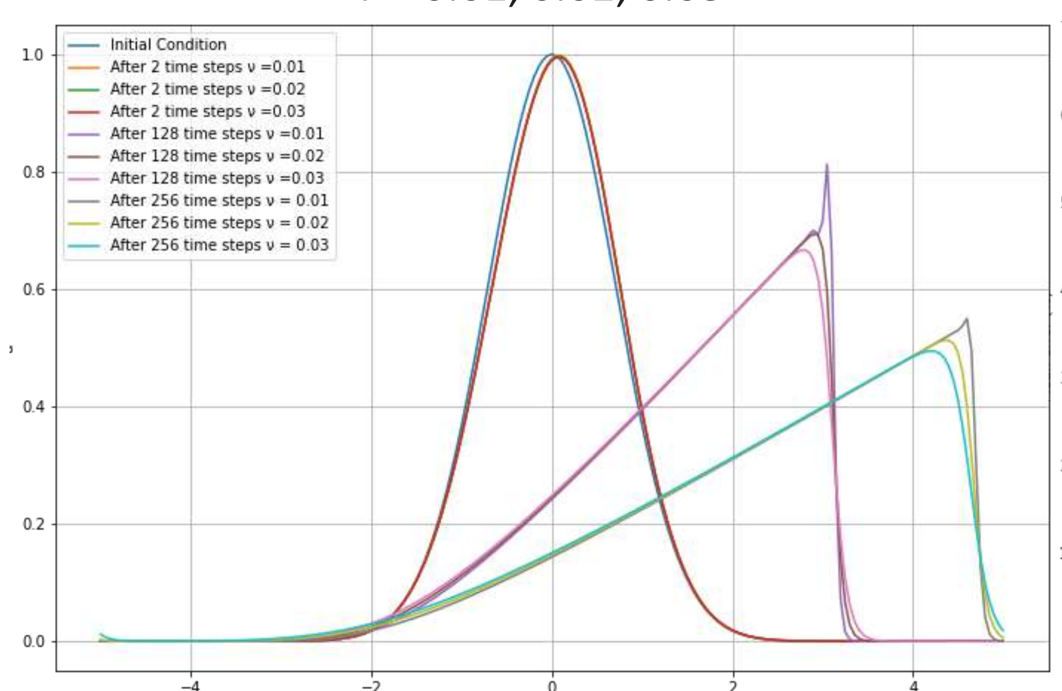
$$u_t = -1.000166uu_x + 0.199643u_{xx}$$

$$u_t = 0.000286 + 0.039955u - 0.296344u^2 - 0.457437u^3 + \cdots$$

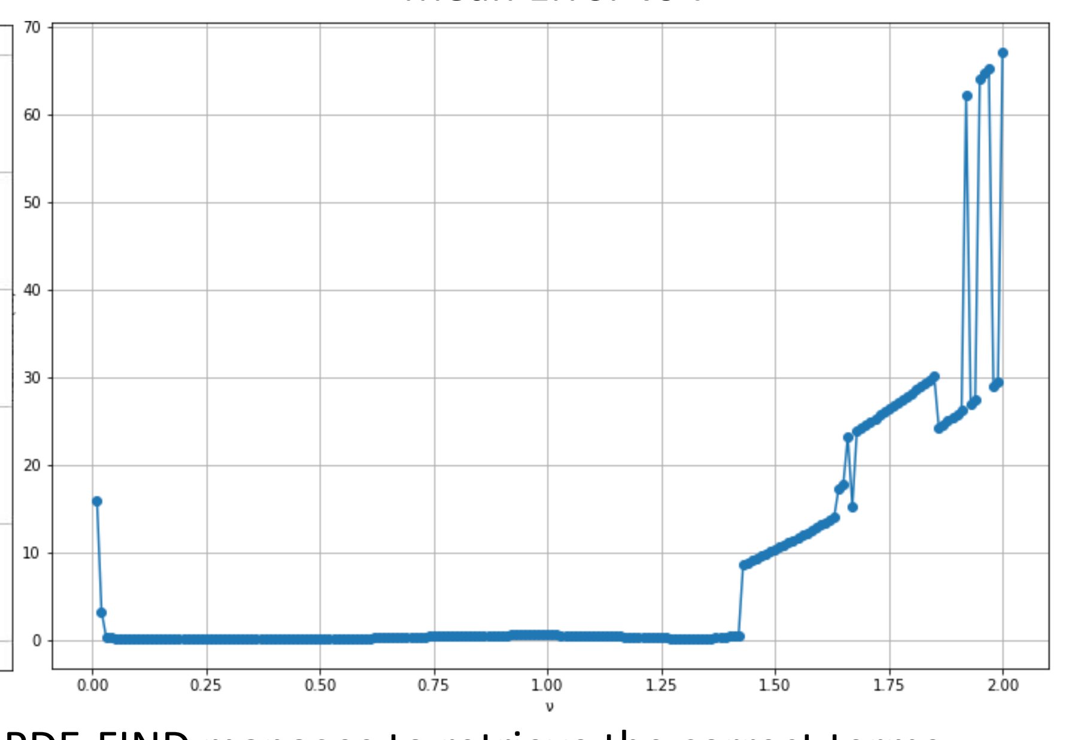
When ν = 0.02, a shock is formed, and PDE-FIND fails to discover the correct terms. When ν = 0.2, the surface is rather smooth and PDE-FIND returns roughly the original equation. When ν = 2, the function diffuses too quickly for PDE-FIND to retrieve the relevant terms. It is natural to conjecture that PDE-FIND performs better when the function is smooth with smaller diffusion term ν. To investigate the condition for PDE-FIND to behave well, we test PDE-FIND on 200 different values of ν = 0.01, …, 2.00, and create a table containing ν, the discovered PDEs, and the parameter errors. Below are selected parts of the table.

ν	PDE	Mean parameter error	Std. of parameter error
0.01	u_t = (0.050140 +0.000000i)u + (-0.163713 +0.000000i)u^2 + (0.100025 +0.000000i)u^3 + …	16.009310%	14.174193%
0.02	u_t = (-1.057625 +0.000000i)uu_{x} + (0.283156 +0.000000i)u^2u_{x} + …	3.319493%	2.442960%
0.03	u_t = (-0.995775 +0.000000i)uu_{x} + (0.029581 +0.000000i)u_{xx}	0.420690%	0.001847%
0.04	u_t = (-0.997450 +0.000000i)uu_{x} + (0.039687 +0.000000i)u_{xx}	0.283914%	0.028941%
…			
1.41	u_t = (-0.995066 +0.000000i)uu_{x} + (1.409464 +0.000000i)u_{xx}	0.514596%	0.021155%
1.42	u_t = (-0.994757 +0.000000i)uu_{x} + (1.419375 +0.000000i)u_{xx}	0.574683%	0.050394%
1.43	u_t = (-0.998046 +0.000000i)uu_{x} + (1.447058 +0.000000i)u_{xx} + (-0.312211 +0.000000i)uu_{xx} + …	8.626920%	8.431511%
1.44	u_t = (-0.997805 +0.000000i)uu_{x} + (1.457516 +0.000000i)u_{xx} + (-0.320027 +0.000000i)uu_{xx} + …	8.867872%	8.648358%
…			
1.99	u_t = (-0.034076 +0.000000i)u + (0.260786 +0.000000i)u^2 + (-0.391764 +0.000000i)u^3 + …	29.460429%	16.816766%
2.00	u_t = (0.000286 +0.000000i) + (-0.039955 +0.000000i)u + (0.296344 +0.000000i)u^2 +…	67.171925%	20.811909%

ν = 0.01, 0.02, 0.03



Mean Error vs ν



The table shows that for ν between 0.01 and 1.42, PDE-FIND manages to retrieve the correct terms, with their mean parameter errors less than 2%. Graphs at the cutoff points shows from ν = 0.02 to ν = 0.03, the function smooths out and PDE-FIND becomes accurate. When ν goes above 1.43, PDE-FIND begins to pick up unrelated terms, and the mean parameter error sees a sharp rise.

Now set ν = 0.20, and try to identify the same dynamic with some added noise. Add a random noise with weighting λ = 10^{-6}, 10^{-5}, … , 0.1, 1 to test the noise-sensitivity of PDE-FIND.

λ	PDE	Mean parameter error	Std. of parameter error
0.000001	u_t = (-1.004325 +0.000000i)uu_{x} + (0.199513 +0.000000i)u_{xx}	0.459872%	0.027403%
0.000010	u_t = (-1.004322 +0.000000i)uu_{x} + (0.199513 +0.000000i)u_{xx}	0.459751%	0.027505%
0.000100	u_t = (-1.004292 +0.000000i)uu_{x} + (0.199496 +0.000000i)u_{xx}	0.466512%	0.037324%
0.001000	u_t = (-1.005010 +0.000000i)uu_{x} + (0.180168 +0.000000i)u_{xx} + …	10.166434%	9.665440%
0.010000	u_t = (-1.002290 +0.000000i)uu_{x} + (0.584189 +0.000000i)uu_{xx} + …	100.114487%	99.885513%
0.100000	u_t = (0.006246 +0.000000i) + (0.038874 +0.000000i)u + (-0.184946 +0.000000i)u^2 + …	122.070662%	77.081559%
1.000000	u_t = (-0.104636 +0.000000i)u + (1.114702 +0.000000i)u^2 + (-2.715334 +0.000000i)u^3 +….	150.000000%	50.000000%

The table shows that PDE-FIND only gives the right result for noise values up to weighting of 10^{-4}, and fails for a bigger weighting index.

Reference & Acknowledgement

[1] Champion, Kathleen, Bethany Lusch, J. Nathan Kutz, and Steven L. Brunton. 2019. "Data-Driven Discovery of Coordinates and Governing Equations." *Proceedings of the National Academy of Sciences* 116 (45): 22445–51. https://doi.org/10.1073/pnas.1906995116.

[2] Rudy, Samuel H., Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz. 2017. "Data-Driven Discovery of Partial Differential Equations." *Science Advances* 3 (4): e1602614. https://doi.org/10.1126/sciadv.1602614.

[3] Wani, Sachin S., and Sarita H. Thakar. 2013. "Crank-Nicolson Type Method for Burgers Equation." *International Journal of Applied Physics and Mathematics*, 324–28. https://doi.org/10.7763/ijapm.2013.v3.230

* When applied to the diffusion equation, FTCS is numerically stable if and only if $\Delta t \leq \frac{\Delta x^2}{2D}$.

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