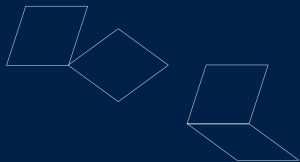


Data-Driven Discovery of Partial Differential Equations

ZIHAN ZHOU

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Partial Differential Equations - Governing a System

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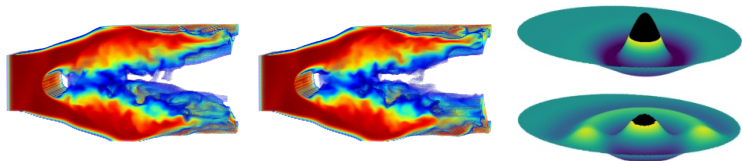


Figure: Left: the 3D Navier-Stokes Equation. Right: the 2D wave equation

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Data-driven PDE discovery

- Suppose we have a dataset for a system regarding a certain quantity u , but the governing PDE for u is unknown. Assume the PDE is of the generic form

$$u_t = F(u, u_x, u_{xx}, \dots, x, \mu), \quad (4)$$

where $F(\cdot)$ is an unknown, usually nonlinear function of $u(x, t)$ and its derivatives, parameterized by μ . Goal: to discover F from the data.

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- Input data** $\mathbf{U} \in \mathbb{C}^{mn}$ is a matrix of values of u collected at m time steps with time interval Δt and n spatial locations with space interval Δx given by

$$\mathbf{U} = \begin{bmatrix} u(0, 0) & \dots & u(n\Delta x, 0) \\ \vdots & & \vdots \\ u(0, m\Delta t) & \dots & u(n\Delta x, m\Delta t) \end{bmatrix}. \quad (5)$$

\mathbf{U} is flattened as a vector $[u(0, 0) \dots u(n\Delta x, 0) \dots u(0, m\Delta t) \dots u(n\Delta x, m\Delta t)]$ of length mn to serve as the input to our the machine learning algorithm.

Discretizing Target PDE and Learning Coefficients

Applying numerical methods (finite difference methods, or polynomial interpolation) to input data \mathbf{U} yields a **dataset** $\mathbf{U}_t \in \mathbb{R}^{mn}$ of **time derivative** u_t . The discrete form of the target PDE $u_t = F(u, u_x, u_{xx}, \dots, x, \mu)$ can thus be written as

$$\mathbf{U}_t = [u_t(0, 0) \dots u_t(n\Delta x, m\Delta t)]^T = \Theta(\mathbf{U}, \mathbf{Q})\xi. \quad (6)$$

Here $\mathbf{Q} \in \mathbb{C}^{mn}$ denotes **additional input**, and $\Theta(\mathbf{U}, \mathbf{Q}) \in \mathbb{C}^{mn \times D}$ is a **library of D candidate terms** and takes the form

$$\Theta(\mathbf{U}, \mathbf{Q}) = [\mathbf{1} \quad \mathbf{U} \quad \mathbf{U}^2 \dots \quad \mathbf{Q} \quad \dots \quad \mathbf{U}_x \quad \mathbf{U}\mathbf{U}_x \quad \dots]. \quad (7)$$

$\xi \in \mathbb{C}^D$ is the **coefficient vector** containing coefficients of each of the candidate terms. We apply machine learning methods to obtain the correct coefficient vector ξ .

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Example (Diffusion Equation)

Suppose the data \mathbf{U} is governed by the 1D heat equation $u_t = u_{xx}$, then we may build a library of $D = 6$ candidate terms

$$\Theta(\mathbf{U}, \mathbf{Q}) = [\mathbf{1} \quad \mathbf{U} \quad \mathbf{U}^2 \quad \mathbf{U}_x \quad \mathbf{U}_{xx} \quad \mathbf{U}\mathbf{U}_x],$$

and if our method is successful, we will get a coefficient vector $\xi \in \mathbb{C}^{D=6}$ that takes the value

$$\xi = [0 \ 0 \ 0 \ 0 \ 1 \ 0]^T.$$

Sparse Regression: Ridge, LASSO, and Elastic Net

Our goal is to find the optimal coefficient vector $\xi \in \mathbb{C}^D$ satisfying

- $\mathbf{U}_t \approx \Theta(\mathbf{U}, \mathbf{Q})\xi$,
- ξ is sparse, so that only the most relevant terms are included.

To achieve this, it is natural to consider applying the sparse regression models

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Three Types of Sparse Regression

- **Ridge Regression:** aims to find $\hat{\xi}$ that minimizes the loss function

$$\hat{\xi} = \operatorname{argmin}_{\xi} L(\xi), \text{ where } L(\xi) = \|\Theta\xi - \mathbf{U}_t\|_2^2 + \lambda\|\xi\|_2, \quad (8)$$

where $\|\xi\|_2 = \sqrt{\xi_1^2 + \cdots + \xi_D^2}$ is the L_2 norm and λ a constant coefficient

- **LASSO Regression:** similar structure, but uses L_1 norm instead of the L_2 norm

$$L(\xi) = \|\Theta\xi - \mathbf{U}_t\|_2^2 + \alpha\|\xi\|_1, \quad (9)$$

where $\|\xi\|_1 = |\xi_1| + \cdots + |\xi_D|$ is the L_1 norm.

- **Elastic Net Regression** simply combines the two regularization terms above:

$$L(\xi) = \|\Theta\xi - \mathbf{U}_t\|_2^2 + \lambda\|\xi\|_2 + \alpha\|\xi\|_1. \quad (10)$$

Minimizing $\|\Theta\xi - \mathbf{U}_t\|_2^2$ fits ξ to the data \mathbf{U}_t , and minimizing $\|\xi\|_1$ and/or $\|\xi\|_2$ shrinks coefficients of irrelevant terms.

Sequential Threshold Ridge Regression

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$$\hat{\xi} = \operatorname{argmin}_{\xi} L(\xi), \text{ where } L(\xi) = \|\Theta(\mathbf{U}, \mathbf{Q})\xi - \mathbf{U}_t\|_2^2 + \epsilon \kappa(\Theta(\mathbf{U}, \mathbf{Q})) \|\xi\|_0. \quad (11)$$

$\|\cdot\|_0$ is the L_0 **norm that counts the number of nonzero elements** in ξ , $\kappa(\Theta(\mathbf{U}, \mathbf{Q}))$ is the **condition number** of the matrix Θ .

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To get the above $\hat{\xi}$, sparse regression is applied with sequential thresholding:

Algorithm 3: Sequential Threshold Ridge Regression:STRidge($\Theta, \mathbf{U}_t, \lambda, tol, \text{iters}, \text{num_big}$)

```
 $\hat{\xi} \leftarrow \operatorname{argmin}_{\xi} (\|\Theta\xi - \mathbf{U}_t\|_2^2 + \lambda\|\xi\|_2)$                                 #standard ridge regression
biginds  $\leftarrow \{j : |\hat{\xi}_j| \geq tol\}$                                 #select indices of large coefficients

#Check if number of big coefficients changed from last time
if num_big  $\neq \text{len}(\text{biginds})$  then
    num_big  $\leftarrow \text{len}(\text{biginds})$                                 #Updates number of big coefficients
     $\hat{\xi}[\sim \text{biginds}] \leftarrow 0$                                     #set small coefficients to 0
     $\hat{\xi}[\text{biginds}] \leftarrow \text{STRidge}(\Theta[:, \text{biginds}], \mathbf{U}_t, \lambda, tol, \text{iters} - 1, \text{num\_big})$ 
                                                                #recursive call with fewer coefficients
else
    return  $\hat{\xi}$ 
end
```

Generating Simulation Data with Finite Difference Method

Let $u_t(x, t) = F(u, u_x, \dots)$, $x \in [0, L]$, $t \in [0, T]$ be a PDE, with initial condition $u(x, 0) = f(x)$, boundary conditions $u(0, t) = g(t)$, $u(L, t) = h(t)$. A simulation dataset for this PDE can be generated using **finite difference methods (FDM)**.

Finite Difference Methods: FTCS and Crank-Nicholson

- **Forward difference in time, central difference for space (FTCS):**

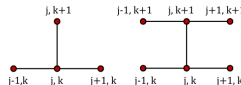
$$U_t \approx \frac{U_j^{k+1} - U_j^k}{\Delta t}, \quad U_x = \frac{U_{j+1}^k - U_{j-1}^k}{2\Delta x}, \quad U_{xx} = \frac{U_{j+1}^k - 2U_j^k + U_{j-1}^k}{2(\Delta x)^2} \quad (12)$$

- **Crank-Nicholson method**, which uses the same formulation of U_t and U_x but

$$UU_x = \frac{1}{2} \left(U_j^k \frac{U_{j+1}^{k+1} - U_{j-1}^k}{2\Delta x} + U_j^{k+1} \frac{U_{j+1}^k - U_{j-1}^k}{2\Delta x} \right) \quad (13)$$

$$U_{xx} \approx \frac{1}{2} \left(\frac{U_{j+1}^{k+1} - 2U_j^{k+1} + U_{j-1}^{k+1}}{2\Delta x} + U_j^{k+1} \frac{U_{j+1}^k - U_{j-1}^k}{2\Delta x} \right) \quad (14)$$

$$\mathbf{U} = \begin{bmatrix} u(0, 0) & \dots & u(n\Delta x, 0) \\ \vdots & & \vdots \\ u(0, m\Delta t) & \dots & u(n\Delta x, m\Delta t) \end{bmatrix} = \begin{bmatrix} U_0^0 & \dots & U_n^0 \\ \vdots & & \vdots \\ U_0^m & \dots & U_n^m \end{bmatrix}$$



Testing results: Linear Advection Equation

We now generate data set with FDM and test the accuracy of the regression algorithm.

The advection equation

The **advection equation** is a hyperbolic equation that represents how a scalar quantity u (such as temperature, concentration, etc.) is transported by a fluid moving with a constant velocity c in a single spatial dimension. For our example we set $c = 1$ and use **Gaussian initial condition** and **periodic boundary condition**.

$$u_t(x, t) = -cu_x(x, t), \quad x \in [-L/2, L/2], t \in [0, T] \quad (15)$$

$$u(x, 0) = \exp(-x^2) \quad , \quad (16)$$

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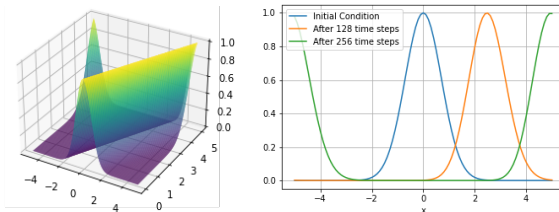
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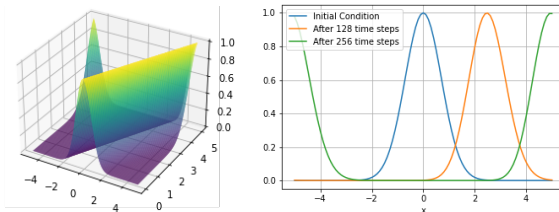
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The PDE discovered by the data-driven method from this dataset is $u_t = -0.999448u_x$.

The Diffusion Equation

The **diffusion equation**, also known as **the 1D heat equation**, describes how heat u (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.

$$u_t = du_{xx}, \quad x \in [-L/2, L/2], t \in [0, T]. \quad (18)$$

For our example we set $d = 0.1$ and apply the same Gaussian initial condition and periodic boundary condition.

Testing results: Diffusion Equation

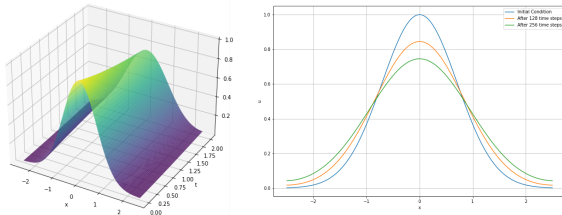
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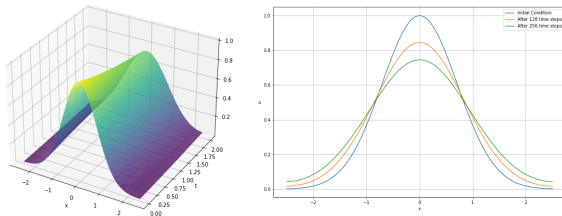
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The PDE discovered by data-driven method from this dataset is $u_t = 0.100003u_{xx}$.

Testing Results: Burger's Equation

Burger's Equation

Burgers' equation is a fundamental PDE from the field of fluid mechanics and can be used for studying shock waves. The equation is given by

$$u_t = -uu_x + \nu u_{xx}, \quad x \in [-L/2, L/2], t \in [0, T], \quad (19)$$

where u represents speed in a fluid flow context, and ν is viscosity.

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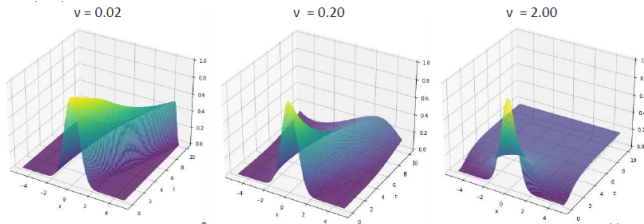
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The simulation results of $u_t = -uu_x + \nu u_{xx}$ by Crank-Nicholson are given below



ν	Discovered PDE
0.02	$u_t = -1.06uu_x + 0.29u^2u_x - 0.26u^3u_x + 0.02u_{xx}$
0.20	$u_t = -uu_x + 0.20u_{xx}$
2.00	$u_t = 0.04u - 0.30u^2 - 0.46u^3 + \dots$

Effect of Smoothness

Previous results show that our method appears to only work for a certain range of viscosity ν . We tested the method on $\nu = 0.01, 0.02, \dots, 2.00$ to investigate the cut-off points.

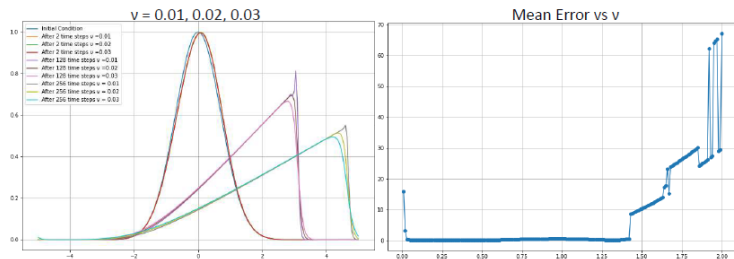
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ν	PDE	Mean parameter error	Std. of parameter error
0.01	$u_t = (0.050140 + 0.000000i)u + (-0.163713 + 0.000000i)u^2 + (0.100025 + 0.000000i)u^3 + \dots$	16.009310%	14.174193%
0.02	$u_t = (-1.057625 + 0.000000i)u u_x + (0.283156 + 0.000000i)u^2 u_x + \dots$	3.319493%	2.442960%
0.03	$u_t = (-0.995775 + 0.000000i)u u_x + (0.029581 + 0.000000i)u_{xx} + \dots$	0.420690%	0.001847%
0.04	$u_t = (-0.997450 + 0.000000i)u u_x + (0.039687 + 0.000000i)u_{xx} + \dots$	0.283914%	0.028941%

1.41	$u_t = (-0.995066 + 0.000000i)u u_x + (1.409464 + 0.000000i)u_{xx} + \dots$	0.514596%	0.021155%
1.42	$u_t = (-0.994757 + 0.000000i)u u_x + (1.419375 + 0.000000i)u_{xx} + \dots$	0.574683%	0.050394%
1.43	$u_t = (-0.998046 + 0.000000i)u u_x + (1.447058 + 0.000000i)u_{xx} + (-0.312211 + 0.000000i)u u_x u_x + \dots$	8.626920%	8.431511%
1.44	$u_t = (-0.997805 + 0.000000i)u u_x + (1.457516 + 0.000000i)u_{xx} + (-0.320027 + 0.000000i)u u_x u_x + \dots$	8.867872%	8.648358%

1.99	$u_t = (-0.034076 + 0.000000i)u + (0.260786 + 0.000000i)u^2 + (-0.391764 + 0.000000i)u^3 + \dots$	29.460429%	16.816766%
2.00	$u_t = (0.000286 + 0.000000i) + (-0.039955 + 0.000000i)u + (0.296344 + 0.000000i)u^2 + \dots$	67.171925%	20.811909%



- $\nu < 0.02$: a shock is formed, does not identify the correct terms.
- $0.02 \leq \nu \leq 1.42$: retrieves the original PDE.
- $\nu \geq 1.43$: diffusing too quickly, does not reflect the dynamics, gets inaccurate results.

Effect of Regression Type

The original paper does not test the model with LASSO and Elastic Net. To fill the blank, I modified the STRidge code to develop the algorithms STLasso and STElasticNet for further exploration.

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ν	Regression Type	Discovered PDE	Runtime (s)	Mean Error (%)	Std Error(%)
2.00	Ridge	$u_t = 2.221u^2u_{xx} - 1.751u^3u_{xx} - 0.009u_{xxx} + 0.060uu_{xxx} \dots$	1.90	67.2	20.8
2.00	LASSO	$u_t = 2.047u_{xx} - 0.750uu_{xx} + 2.284u^2u_{xx} - 1.792u^3u_{xx} \dots$	37.88	29.9	17.1
2.00	Elastic Net	$u_t = 2.047u_{xx} - 0.750uu_{xx} + 2.284u^2u_{xx} - 1.792u^3u_{xx} \dots$	8.61	29.9	17.1
0.20	Ridge	$u_t = -1.00uu_x + 0.200u_{xx}$	1.2	0.1	0.1
0.20	LASSO	$u_t = -1.00uu_x + 0.200u_{xx}$	7.0	0.1	0.1
0.20	Elastic Net	$u_t = -1.00uu_x + 0.200u_{xx}$	8.9	0.1	0.1
0.02	Ridge	$u_t = -0.040u + 0.296u^2 - 0.457u^3 + 0.057u_x - 1.880uu_x + \dots$	3.0	742.9	2429.8
0.02	LASSO	$u_t = -0.035u + 0.266u^2 - 0.402u^3 - 1.128uu_x + 1.411u^2u_x \dots$	18.8	701.4	2437.6
0.02	Elastic Net	$u_t = -0.035u + 0.266u^2 - 0.402u^3 - 1.128uu_x + 1.411u^2u_x \dots$	18.7	701.4	2437.6

Conclusion







- The data-driven method works well when the data is smooth and no shock waves are formed.
- Ridge regression is the most efficient compared to the other two sparse regressions, and accuracy does not seem to differ.
- (Not included in this presentation) Accuracy suffers when a certain level of noise is introduced.



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Related Works

- More on machine learning for PDE-discovery:
 - Brunton et al., *"Discovering governing equations from data by sparse identification of nonlinear dynamical systems"* (2016)
 - Baddoo et al., *"Physics-informed dynamic mode decomposition"* (2023)
- Physics-Informed Neural Networks (PINN) for PDE-discovery:
 - Raissi et al., *"Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations"* (2019)
 - Chen et al., *"Physics-informed learning of governing equations from scarce data"* (2021)
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