

Finding a Universal Model of Nonlinear Pattern Forming PDEs in terms of the Phase Parameter

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Motivation

- ▶ We are interested in pattern forming systems, characterized by modulated stripe patterns. The canonical example of such patterns is Rayleigh-Bénard convection.
- ▶ Such patterns are observed as solutions to various non-linear PDEs.
- ▶ However they are thought to all obey a universal diffusion equation in terms of the *phase* of the pattern. We would like to derive such an equation.

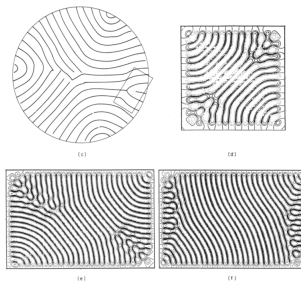


Fig. 1. Configuration of convective cells in large aspect ratio cells. (a) and (b) are from the work of Gollub et al. (1972) and (c) and (d) are from the work of Gollub et al. (1972).

Cross-Newell Phase Diffusion Equation

- ▶ Many nonlinear PDEs admit an exact straight roll solution of the form

$$w = F(\theta = \vec{k} \cdot \vec{x}, A) = \sum A_n(k) \cos n\theta.$$

- ▶ For most natural patterns, the wave number $k = |\vec{k}|$ is not constant, but varies slowly over the box. So we seek a solution where the wave number is slowly modulating over the box

$$w = F(\theta = \frac{1}{\epsilon} \Theta(\vec{X} = \epsilon \vec{x}, T = \epsilon^2 t) = \frac{1}{\epsilon} \int \vec{k} d\vec{X}) + \epsilon w_1 + \dots$$

- ▶ Using this ansatz, and imposing some restrictive assumptions, one can show that the phase Θ obeys the Cross-Newell equation

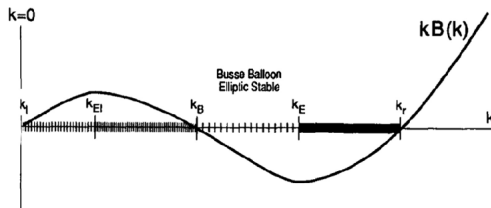
$$\tau(k) \frac{\partial \Theta}{\partial T} = -\nabla \vec{k} B(k) - \epsilon^2 \eta \nabla^4 \Theta.$$

Cross-Newell as Regularization of a Diffusion Equation

- ▶ The Cross-Newell equation can be written as

$$\tau(k) \frac{\partial \Theta}{\partial T} = -\nabla^2 \Theta B(k) - \epsilon^2 \eta \nabla^4 \Theta.$$

- ▶ The quantities $B(k), (kB(k))'$ determine whether or not $\tau(k) \frac{\partial \Theta}{\partial T} = -\nabla^2 \Theta B(k)$ is ill-posed. It turns out that this is a proper diffusion equation only for $k_B < k < K_E$.
- ▶ For most natural patterns, the preferred wave number k is something like $k_b - c$, ie, just to the left of K_B .
- ▶ Thus, the biharmonic term is added to make the PDE well-posed.



Cross-Newell Equation as variation of Energy

- ▶ Cross-Newell can be expressed as

$$-\frac{\delta F}{\delta \Theta} = \tau(k) \frac{\partial \Theta}{\partial T}$$
$$\epsilon F = \int (1 - |\nabla \Theta|^2)^2 d\vec{X} + \epsilon^2 \int (\nabla^2 \Theta)^2.$$

- ▶ The left term measures energy due to stretching, the right term measures energy due to bending.
- ▶ If we look for "self-dual" solutions by "balancing" the bending energy with the stretching energy, then such solutions solve the Cross-Newell equation if the Gaussian curvature of the solution is 0.
- ▶ For a range of pattern defects/instabilities, one can associate a cost given by the energy functional.

Bringing in some Machine Learning

- ▶ The Cross-Newell equation is limited in the pattern defects it can predict.
- ▶ It's derivation dates back to the 80s, and there has been no proposed modification to capture more patterns.
- ▶ I want to use some data driven methods to analyze this problem.
- ▶ I am starting with simple methods for data driven discovery of PDEs.
- ▶ I will learn how to "rediscover" known non-linear PDEs that generate patterns of interest, and then concoct an experiment to propose governing equations of the corresponding phase surfaces.

PDE Discovery via Sparse Optimization

- ▶ I combined ideas from Kutz et. al. and Hayden Schaeffer for finding governing equations via sparse regression.
- ▶ Suppose we have access to solutions $u(x, y, t)$ on a spatio-temporal grid, and in addition, we are able to estimate time derivatives for each solution, $u_t(x, y, t)$. Let us collect the time derivatives one vector, U_t .
- ▶ We can then form a feature matrix of tall, skinny feature vectors:

$$F_u(t) = \begin{bmatrix} | & | & | & | & | & | & | & | & \dots \\ 1 & u & u^2 & u_x & u_x^2 & uu_x & u_x x & u_x x & \dots \\ | & | & | & | & | & | & | & | & \dots \end{bmatrix}$$

- ▶ We then approximate a solution of

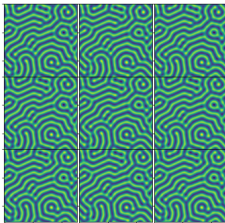
$$\xi = \operatorname{argmin} \|F_u(t)\xi - U_t\|_2^2 + \lambda \|\xi\|_0$$

"Discovering" Swift Hohenberg

- ▶ I used Operator Splitting and Exponential Time Differencing to obtain numerical solutions of Swift-Hohenberg
$$u_t = -\Delta^2 u - 2\Delta u + (R - 1)u - u^3.$$
- ▶ I used backward finite differences for my time derivatives, and spectral derivatives for all spatial derivatives.
- ▶ I used a "coarse" grid for sampling. I.e, I took 20 time steps, and down sampled the spatial grids by a factor of 8.
- ▶ I used Sequentially Thresholded Ridge Regression. This is an iterative method which solve
$$\xi = \operatorname{argmin} \|F_u(t)\xi - U_t\|_2^2 + \lambda \|\xi\|_2^2$$
at each step, and applies a "hard" threshold to coefficients below a certain size, before repeating. The threshold tolerance is determined empirically by using an 80/20 test/train split. We used $\lambda = 1e - 5$.

"Discovering" Swift Hohenberg cont.

► Notebook Demo



Algorithm 1: STRidge($\Theta, \mathbf{U}_t, \lambda, tol, \text{iters}$)

$\hat{\xi} = \arg \min_{\xi} \|\Theta \xi - \mathbf{U}_t\|_2^2 + \lambda \|\xi\|_2^2$ # ridge regression

$\text{bigcoeffs} = \{j : |\hat{\xi}_j| \geq tol\}$ # select large coefficients

$\hat{\xi}[\sim \text{bigcoeffs}] = 0$ # apply hard threshold

$\hat{\xi}[\text{bigcoeffs}] = \text{STRidge}(\Theta[:, \text{bigcoeffs}], \mathbf{U}_t, tol, \text{iters} - 1)$

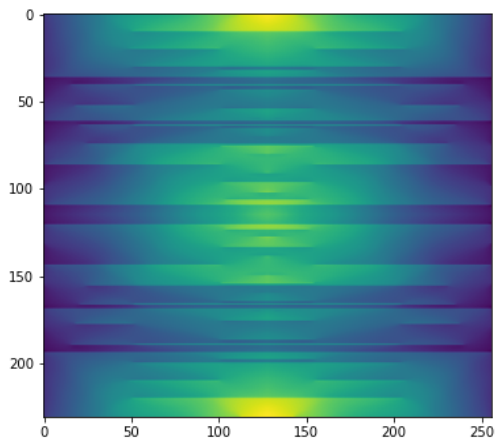
recursive call with fewer coefficients

return $\hat{\xi}$

Next Steps

- ▶ Having successfully "rediscovered" Swift-Hohenberg, I am ready to extend the method to analyze the Cross-Newell Equation.
- ▶ A simple first experiment would be to generate Swift-Hohenberg solutions that obey the restrictions imposed in the Cross-Newell derivation. If I can generate phase surfaces from the solutions, I can run the experiment on the phase surfaces, and see if such an experiment predicts Cross-Newell.
- ▶ It would be neat to derive Cross-Newell, or a variant of it, directly from temperature surface simulations. I am wondering if there is a way to combine a neural network, or other machine learning technique to make this work.
- ▶ First step is to find a reliable method for estimating phase surfaces, and return to the mathematical analysis to understand the Cross-Newell limitations.

Phase Surface Depiction



References

- ▶ MC Cross and Alan C Newell. Convection patterns in large aspect ratio systems. 1984
- ▶ Alan C. Newell and Shankar C. Venkataramani. The universal behavior of modulated stripe patterns 2022
- ▶ Kutz Et. Al. Data-driven discovery of partial differential equations. 2017
- ▶ Hayden Schaeffer Learning partial differential equations via data discovery and sparse optimization, 2017
- ▶ My Codes