A Bayesian Approach for Data-Driven Dynamic Equation Discovery

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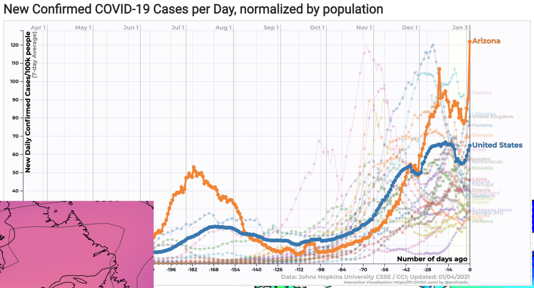
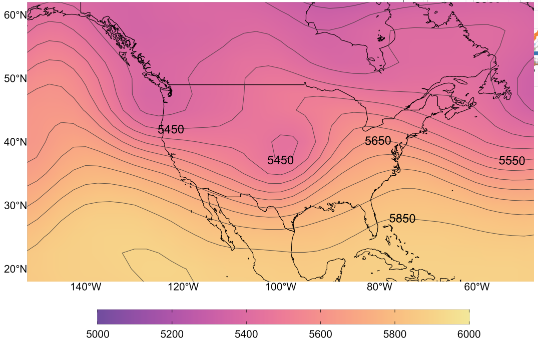
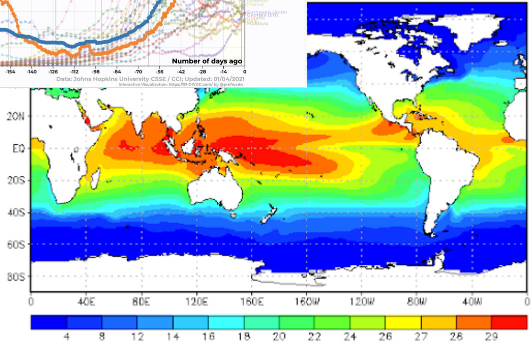
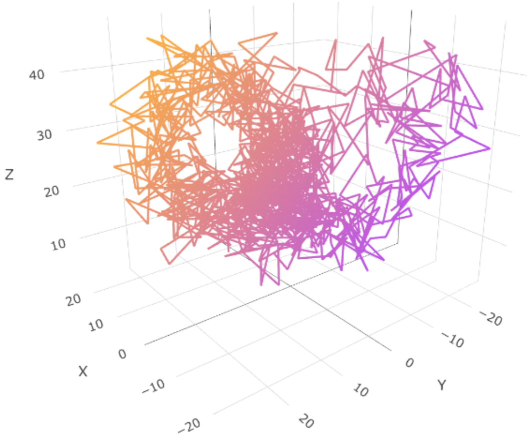
Motivation - Dynamics







Discover the governing equation(s) that define the dynamic system



$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = x(\rho - z) - y$$
$$\frac{dz}{dt} = xy - \beta z$$

Who else has done this?

- **Symbolic Regression** (Bongard and Lipson, 2007; Schmidt and Lipson, 2009; Maslyaev et al., 2019)
  - Search over mathematical expressions (e.g., $+, -, \times$) to find the optimal model; very flexible; computationally expensive; doesn't scale well
- **Sparse Regression** (Brunton et al., 2016; Rudy et al., 2017; Champion et al., 2020)
  - Sparse Identification of Nonlinear Dynamics (SINDy): Three Steps; Requires a *library* of potential functions; very fast
  - Stochastic processes (Boninsegna et al., 2018); Numerical improvement (Schaeffer, 2017; Schaeffer et al., 2018); Python package (*pySINDy*; de Silva et al., 2020)
- **Deep Models**
  - Sparse Regression (Lagergren et al., 2020; Both et al., 2021)
  - Symbolic Regression (Long et al., 2019; Atkinson et al., 2019; Xu et al., 2021)

Statistical Approaches?

- **Bayesian** (Zhang and Lin, 2018; Niven et al., 2020; Yang et al., 2020; Hirsh et al., 2021)
  - Prior on parameters
  - Bayesian differentiable programming
- **Bootstrap** (Fasel et al., 2021)
  - Observations
  - Library terms

- Requires derivatives (e.g., numerical differentiation)
- Observational uncertainty?
- Uncertainty in the dynamic system (e.g., derivatives)

Our Approach

- Bayesian hierarchical modeling: data, process, parameter models
  - **Consider dynamic process to be latent**
  - Accounts for measurement uncertainty and missing data in a probabilistic manner
  - Accounts for process dependence
  - Dynamic system as a random process
- Important components
  - Compute derivatives analytically via basis function representation
  - Feature library
  - Inclusion probability

Notation

Tensor

- $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \ldots \times I_N}$ be a tensor of order N
- n-mode matricization is $\mathbf{X}_{(n)}$: arrange the mode-n fibers to be columns
  - For example, if $\mathcal{Y} \in \mathbb{R}^{I \times J \times K}$, then $\mathbf{Y}_{(3)} \in \mathbb{R}^{K \times (I \times J)}$
  - Generally only concerned with the mode-3 matricization of a tensor and use $\mathbf{Y}$ in place of $\mathbf{Y}_{(3)}$
- The n-mode product of the tensor $\mathcal{X}$ and matrix $\mathbf{B} \in \mathbb{R}^{I_n \times J}$ is $\mathcal{X} \times_n \mathbf{B}$ and is of size $I_1 \times I_2 \ldots \times I_{n-1} \times J \times I_{n+1} \times \ldots \times I_N$
  - $\mathcal{Z} = \mathcal{X} \times_n \mathbf{B} \Leftrightarrow \mathbf{Z}_{(n)} = \mathbf{B}\mathbf{X}_{(n)}$

Derivatives

- Denote partial derivatives using a subscript (e.g., $\frac{\partial u}{\partial t} = u_t$)
- Denote the ith order of a derivative generally as $\frac{\partial^{(i)} u}{\partial t^{(i)}} = u_{t^{(i)}}$

Dynamic System

Consider the dynamic system describing the evolution of a continuous process $\{\mathbf{u}(\mathbf{s}, t) : \mathbf{s} \in D_s, t \in D_t\}$:

$$\mathbf{u}_{t^{(J)}}(\mathbf{s}, t) = M\left(\mathbf{u}(\mathbf{s}, t), \mathbf{u}_x(\mathbf{s}, t), ..., \mathbf{u}_{t^{(1)}}(\mathbf{s}, t), ..., \mathbf{u}_{t^{(J-1)}}(\mathbf{s}, t), \boldsymbol{\omega}(\mathbf{s}, t)\right), \ \mathbf{u}(\mathbf{s}, t) \in \mathbb{R}^N$$

Re-parameterizing and accounting for potential stochastic forcing:

$$\mathbf{u}_{t^{(J)}}(\mathbf{s}, t) = \mathbf{Mf}\left(\mathbf{u}(\mathbf{s}, t), \mathbf{u}_x(\mathbf{s}, t), ..., \mathbf{u}_{t^{(1)}}(\mathbf{s}, t), ..., \boldsymbol{\omega}(\mathbf{s}, t)\right) + \boldsymbol{\eta}(\mathbf{s}, t),$$

- $\mathbf{M}$ is a $N \times D$ *sparse* matrix of coefficients
- $\mathbf{f}(\cdot)$ is a length-D vector-valued nonlinear transformation function
- $\boldsymbol{\eta}(\mathbf{s}, t) \overset{\text{i.i.d.}}{\sim} N(\mathbf{0}, \boldsymbol{\Sigma}_U)$ is a mean zero Gaussian process with variance/covariance matrix $\boldsymbol{\Sigma}_U$

Tensor Formulation of the Dynamic System

$$\mathcal{U}_{t(J)} = \mathcal{F} \times_3 \mathbf{M} + \widetilde{\boldsymbol{\eta}}$$

- Tensor of the dynamic process:
  $\mathcal{U} = \{u(\mathbf{s}, t, n) : \mathbf{s} \in D_s, t = 1, ..., T, n = 1, ..., N\} \in \mathbb{R}^{S \times T \times N}$
- Tensor of the function: $\mathcal{F} \in \mathbb{R}^{S \times T \times D}$ (note, still a function of the state process $\mathcal{U}$)
- Space-time uncertainty tensor: $\widetilde{\boldsymbol{\eta}} \in \mathbb{R}^{S \times T \times N}$

Basis Function Representation

$$\mathcal{U} \approx \sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R} a(p,q,r)\boldsymbol{\psi}(p) \circ \boldsymbol{\phi}(q) \circ \boldsymbol{\theta}(r)$$
$$= \mathcal{A} \times_1 \boldsymbol{\Psi} \times_2 \boldsymbol{\Phi} \times_3 \boldsymbol{\Theta} := [\![\mathcal{A}; \boldsymbol{\Psi}, \boldsymbol{\Phi}, \boldsymbol{\Theta}]\!]$$

- Basis Coefficients: $\mathcal{A} \in \mathbb{R}^{P \times Q \times R}$
- Spatial Basis Functions (fixed, known, differentiable): $\boldsymbol{\Psi} \in \mathbb{R}^{S \times P}$
- Temporal Basis Functions (fixed, known, differentiable): $\boldsymbol{\Phi} \in \mathbb{R}^{T \times Q}$
- Component Basis Functions (fixed, known): $\boldsymbol{\Theta} \in \mathbb{R}^{N \times R}$

$$\mathcal{U}_t = \mathcal{A} \times_1 \boldsymbol{\Psi} \times_2 \boldsymbol{\Phi}_t \times_3 \boldsymbol{\Theta} = [\![\mathcal{A}; \boldsymbol{\Psi}, \boldsymbol{\Phi}_t, \boldsymbol{\Theta}]\!]$$
$$\mathcal{U}_x = \mathcal{A} \times_1 \boldsymbol{\Psi}_x \times_2 \boldsymbol{\Phi} \times_3 \boldsymbol{\Theta} = [\![\mathcal{A}; \boldsymbol{\Psi}_x, \boldsymbol{\Phi}, \boldsymbol{\Theta}]\!]$$
$$\mathcal{U}_{xyt} = \mathcal{A} \times_1 \boldsymbol{\Psi}_{xy} \times_2 \boldsymbol{\Phi}_t \times_3 \boldsymbol{\Theta} = [\![\mathcal{A}; \boldsymbol{\Psi}_{xy}, \boldsymbol{\Phi}, \boldsymbol{\Theta}]\!]$$

Basis Function Representation

Proposition 1

The mode-3 decomposition of $[\![\mathcal{A}; \boldsymbol{\Psi}, \boldsymbol{\Phi}_{t(J)}, \boldsymbol{\Theta}]\!] = \mathcal{F} \times_3 \mathbf{M} + \widetilde{\boldsymbol{\eta}}$ where $\boldsymbol{\eta}(\mathbf{s}, t) \overset{i.i.d.}{\sim} N_N(\mathbf{0}, \Sigma_U)$ in space and time at location $\mathbf{s}$ and time t is

$$\boldsymbol{\Theta}\mathbf{A}(\phi_{t(J)}(t) \otimes \psi(\mathbf{s}))' = \mathbf{M}\mathbf{f}(\mathbf{A}, \psi(\mathbf{s}), \psi_x(\mathbf{s}), ..., \phi_{t(0)}(t), ..., \boldsymbol{\omega}(\mathbf{s}, t)) + \boldsymbol{\eta}(\mathbf{s}, t),$$

where $\mathbf{A}$ is a $R \times PQ$ matrix of basis coefficients, $\psi(\mathbf{s})$ is a length-P vector of spatial basis functions, $\phi(t)$ is a length-Q vector of temporal basis functions, and $\boldsymbol{\Theta}$ is a $N \times R$ matrix of component basis functions.

Space-Time Response

What about equations with a spatio-temporal derivative of $\mathbf{u}$?

$$\nabla^2 \mathbf{u}_t(\mathbf{s}, t) = \mathbf{u}_{xxt}(\mathbf{s}, t) + \mathbf{u}_{yyt}(\mathbf{s}, t)$$

General PDE

$$g(\mathbf{u}_{t^{(J)}}(\mathbf{s}, t)) = M\left(\mathbf{u}(\mathbf{s}, t), \mathbf{u}_x(\mathbf{s}, t), \mathbf{u}_y(\mathbf{s}, t), ..., \mathbf{u}_{t^{(1)}}(\mathbf{s}, t), ..., \boldsymbol{\omega}(\mathbf{s}, t)\right)$$

- $g(\cdot)$ is some linear differential operator
- Fluid dynamics

General Basis Function Representation

Proposition 2

Let $g(\cdot)$ be a linear differential operator. The basis formulation of a PDE with a space-time response $g(\mathbf{u}_{t^{(J)}}(\mathbf{s}, t))$ is

$$\boldsymbol{\Theta}\mathbf{A}(\phi_{t^{(J)}}(t) \otimes g(\psi(\mathbf{s})))'.$$

The general form of a PDE with a spatio-temporal response:

$$\boldsymbol{\Theta}\mathbf{A}(\phi_{t^{(J)}}(t) \otimes g(\psi(\mathbf{s})))' = \mathbf{M}\mathbf{f}(\mathbf{A}, \psi(\mathbf{s}), \psi_x(\mathbf{s}), \phi_{t^{(0)}}(t), \dots) + \boldsymbol{\eta}(\mathbf{s}, t), \quad \boldsymbol{\eta}(\mathbf{s}, t) \overset{i.i.d.}{\sim} N_N(\mathbf{0}, \Sigma_U)$$

$$\nabla^2 \mathbf{u}_t(\mathbf{s}, t) = \mathbf{u}_{xxt}(\mathbf{s}, t) + \mathbf{u}_{yyt}(\mathbf{s}, t) \Rightarrow \boldsymbol{\Theta}\mathbf{A}(\phi_{t^{(1)}}(t) \otimes (\psi_{xx}(\mathbf{s}) + \psi_{yy}(\mathbf{s})))'$$

Hierarchical Model

For location $\mathbf{s}$ and time t, the general model is

$$\begin{aligned}\mathbf{v}(\mathbf{s}, t) &= \mathbf{H}(\mathbf{s}, t)\mathbf{\Theta A}(\phi_{t^{(0)}}(t) \otimes \psi(\mathbf{s}))' + \epsilon(\mathbf{s}, t) \\ \mathbf{\Theta A}(\phi_{t^{(J)}}(t) \otimes g(\psi(\mathbf{s})))' &= \mathbf{Mf}(\mathbf{A}, \psi(\mathbf{s}), \psi_x(\mathbf{s}), \phi_{t^{(0)}}(t), \ldots) + \boldsymbol{\eta}(\mathbf{s}, t)\end{aligned}$$

- $\mathbf{v}(\mathbf{s}, t) \in \mathbb{R}^{L(\mathbf{s},t)}$ is the observed process
- $\mathbf{H}(\mathbf{s}, t) \in \mathbb{R}^{L(\mathbf{s},t)\times N}$ is the incidence matrix
- $\mathbf{M}$ is the $N \times D$ coefficient matrix - Spike and Slab (George et al., 1993)
- $\mathbf{A}$ is the matrix (tensor) of basis coefficients - Elastic Net (Li and Lin, 2010)
- $\epsilon(\mathbf{s}, t) \overset{indep.}{\sim} N_{L(\mathbf{s},t)}(\mathbf{0}, \mathbf{\Sigma}_V(\mathbf{s}, t))$ is the measurement error
- $\boldsymbol{\eta}(\mathbf{s}, t) \overset{i.i.d.}{\sim} N_N(\mathbf{0}, \mathbf{\Sigma}_U)$ is the process error

Simulations and Examples - PDE

Simulations

1. Burgers' Equation
2. Reaction-Diffusion Equation

Examples

1. Barotropic Vorticity Equation

$$\mathbf{v}(\mathbf{s}, t) = \mathbf{u}(\mathbf{s}, t) + \zeta \boldsymbol{\epsilon}(\mathbf{s}, t), \quad \boldsymbol{\epsilon}(\mathbf{s}, t) \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_N)$$

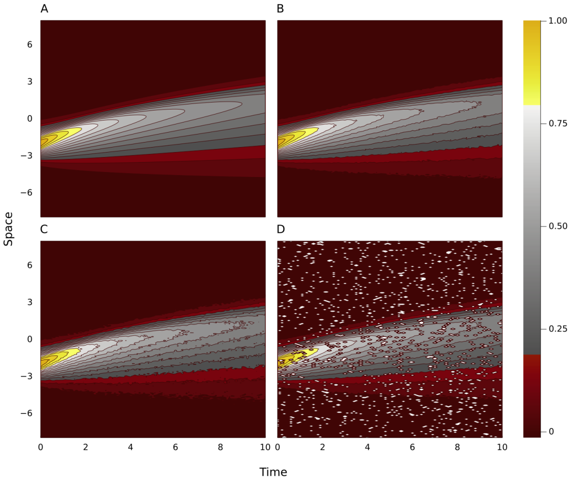
- $\mathbf{u}(\mathbf{s}, t)$ is the simulated data
- σ is the standard deviation of $\mathbf{u}(\mathbf{s}, t)$
- $\zeta \in [0, 1]$ is the percent of noise

Burgers' Equation

$$u_t(x,t) = -u(x,t)u_x(x,t) + \nu u_{xx}(x,t)$$
$$u(x,0) = exp\{-(x+2)^2\}$$

- $\nu = 0.1$ is the viscocity
- (A) no measurement noise
  (B) 2% measurement noise
  (C) 5% measurement noise
  (D) 2% measurement noise with 5% of data missing at random

$$[u, u^2, u^3, u_x, uu_x, u^2u_x, u^3u_x, u_{xx}, uu_{xx}, u^2u_{xx}, u^3u_{xx}, u_{xxx}, uu_{xxx}, u^2u_{xxx}, u^3u_{xxx}]$$



Burgers' Equation

Noise	Missing Data	Statistic	Discovered Equation
0%	0%	Mean	$u_t = -\mathbf{0.994}uu_x + \mathbf{0.098}u_{xx}$
		Lower HPD	$u_t = -1.022uu_x + 0.092u_{xx}$
		Upper HPD	$u_t = -0.964uu_x + 0.103u_{xx}$
2%	0%	Mean	$u_t = -\mathbf{0.990}uu_x + \mathbf{0.096}u_{xx}$
		Lower HPD	$u_t = -1.033uu_x + 0.086u_{xx}$
		Upper HPD	$u_t = -0.954uu_x + 0.103u_{xx}$
5%	0%	Mean	$u_t = -\mathbf{0.981}uu_x + 0.094u_{xx}$
		Lower HPD	$u_t = -1.022uu_x + 0.087u_{xx}$
		Upper HPD	$u_t = -0.951uu_x + 0.099u_{xx}$
2%	5%	Mean	$u_t = -\mathbf{0.957}uu_x + 0.087u_{xx}$
		Lower HPD	$u_t = -1.003uu_x + 0.078u_{xx}$
		Upper HPD	$u_t = -0.931uu_x + 0.095u_{xx}$

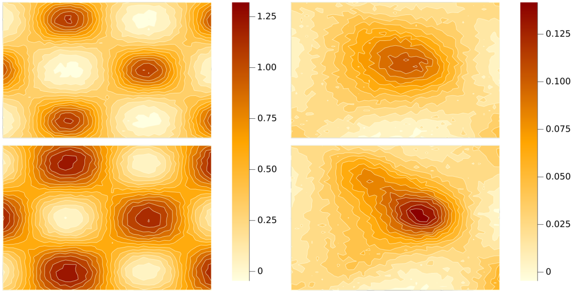
$$u_t = -uu_x + 0.1u_{xx}$$

Reaction-Diffusion Equation

$$u_t = D_u u_{xx} + D_u u_{yy} + \gamma_0 u - \frac{\gamma_0}{\gamma_1} u^2 - \beta uv \qquad u(\mathbf{s}, 0) = \exp\{cos(2\pi x/15) sin(2\pi y/15)\}$$

$$v_t = D_v v_{xx} + D_v v_{yy} + \mu uv - \eta v \qquad v(\mathbf{s}, 0) = 0.1 \exp\{cos(2\pi y/30) sin(2\pi x/30 - 5)\}$$

- $D = 0.1$ is the diffusivity constant
- Predator-prey reaction component
- Prey (left) and predator (right) with 5% measurement noise



$$[u, u^2, u^3, v, v^2, v^3, uv, u^2v, uv^2, uu_x, uu_y, vv_x,$$
$$vv_y, u_x, u_y, u_{xx}, u_{yy}, u_{xy}, v_x, v_y, v_{xx}, v_{yy}, v_{xy}]$$

Reaction-Diffusion Equation

Noise	Statistic	Recovered Equation
5%	Mean	$u_t = \mathbf{0.401}u - 0.269u^2 - \mathbf{0.493}uv + 0.090u_{xx} + \mathbf{0.099}u_{yy}$
	Lower HPD	$u_t = 0.400u - 0.270u^2 - 0.504uv + 0.085u_{xx} + 0.091u_{yy}$
	Upper HPD	$u_t = 0.403u - 0.267u^2 - 0.487uv + 0.093u_{xx} + 0.102u_{yy}$
5%	Mean	$v_t = -\mathbf{0.101}v + \mathbf{0.300}uv + 0.092v_{xx} + \mathbf{0.106}v_{yy}$
	Lower HPD	$v_t = -0.103v + 0.297uv + 0.086v_{xx} + 0.097v_{yy}$
	Upper HPD	$v_t = -0.099v + 0.302uv + 0.095v_{xx} + 0.151v_{yy}$

$$u_t = 0.4u - 0.266u^2 - 0.5uv + 0.1u_{xx} + 0.1u_{yy}$$
$$v_t = -0.1v + 0.3uv + 0.1v_{xx} + 0.1v_{yy}$$

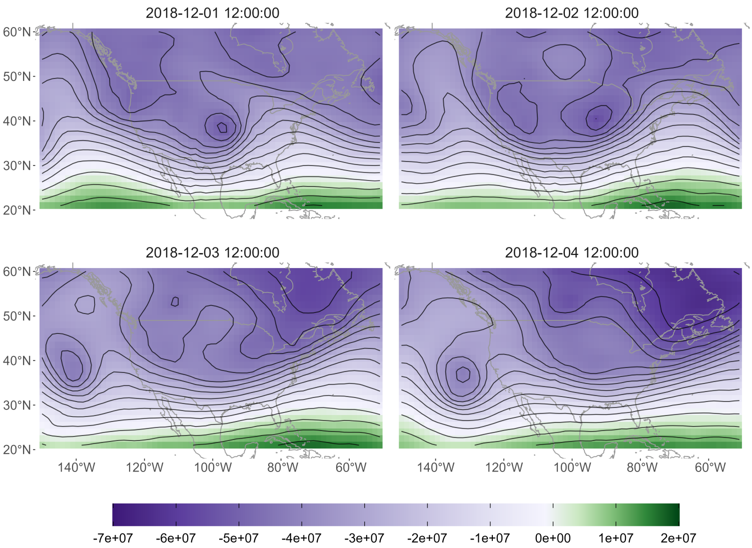
Barotropic Vorticity Equation

$$\xi_t(\mathbf{s}, t) = -\mathbf{v}(\mathbf{s}, t) \cdot \nabla(\xi(\mathbf{s}, t) + f(\phi(\mathbf{s})))$$

- $\xi = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \nabla^2 \psi$ is the relative vorticity
- $\mathbf{v} = (u, v)$ is the non-divergent horizontal wind
- $u = -\frac{\partial \psi}{\partial y}$ is the Zonal wind, $v = \frac{\partial \psi}{\partial x}$ is the Meridional wind
- $f = 2\Omega sin(\phi)$ is the Coriolis parameter with $\Omega = 7.292 \times 10^{-5}$ rad s^{-1} the angular speed of rotation of the Earth
- ψ is the streamfunction

$$\nabla^2 \psi_t = \psi_{xxt} + \psi_{yyt} = \psi_y \psi_{xxx} + \psi_y \psi_{xyy} - \psi_x \psi_{xxy} - \psi_x \psi_{yyy} - \psi_x f_y$$

Barotropic Vorticity Equation



Streamfunction is a computed quantity based on the observed geopotential height, Φ

$$\psi(\mathbf{s}, t) = \Phi^*(\mathbf{s}, t)/f(\phi(\mathbf{s}))$$

$$\Phi^*(\mathbf{s}, t) = \Phi(\mathbf{s}, t) - \int_D \Phi(\mathbf{s}, t)$$

Barotropic Vorticity Equation

$$[\psi, \psi_x, \psi_{xx}, \psi_y, \psi_{yy}, \psi_{xy}, \psi_x\psi_{xxx}, \psi_y\psi_{xxx}, \psi_x\psi_{yyy}, \psi_y\psi_{yyy},$$
$$\psi_x\psi_{xxy}, \psi_y\psi_{xxy}, \psi_x\psi_{xyy}, \psi_y\psi_{xyy}, \psi_x f_y, \psi_y f_y]$$

	Discovered Equation
Mean	$\nabla^2\psi_t = \mathbf{0.289}\psi_y\psi_{xxx} + \mathbf{0.277}\psi_y\psi_{xyy} - \mathbf{0.280}\psi_x\psi_{xxy} - \mathbf{0.185}\psi_x\psi_{yyy} - 6.354\psi_x f_y$
Lower HPD	$\nabla^2\psi_t = 0.235\psi_y\psi_{xxx} + 0.267\psi_y\psi_{xyy} - 0.343\psi_x\psi_{xxy} - 0.215\psi_x\psi_{yyy} - 7.570\psi_x f_y$
Upper HPD	$\nabla^2\psi_t = 0.317\psi_y\psi_{xxx} + 0.286\psi_y\psi_{xyy} - 0.223\psi_x\psi_{xxy} - 0.160\psi_x\psi_{yyy} + 1.491\psi_x f_y$

$$\nabla^2\psi_t = \psi_y\psi_{xxx} + \psi_y\psi_{xyy} - \psi_x\psi_{xxy} - \psi_x\psi_{yyy} - \psi_x f_y$$

Contributions

- Bayesian hierarchical method to learn complex nonlinear dynamic equations using a data-driven approach
- Robust to measurement noise and missing data
- Provide uncertainty quantification and inclusion probabilities to the terms in the library
- Bypass the need for numerical differentiation

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