Along the **SINDy** Frontier

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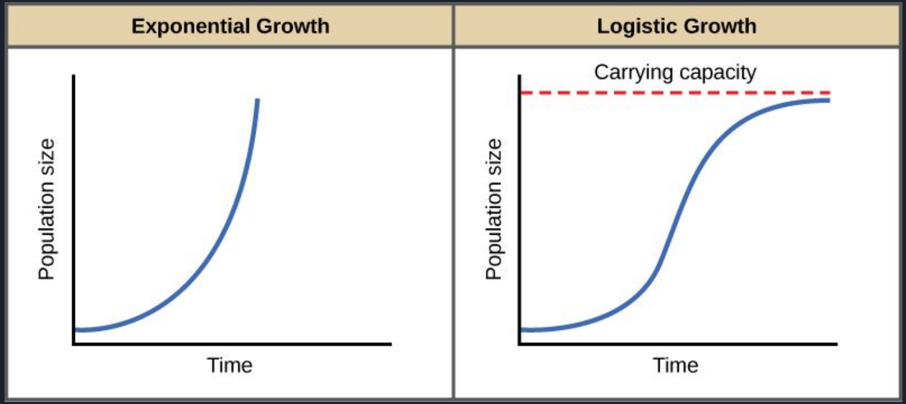
Overview

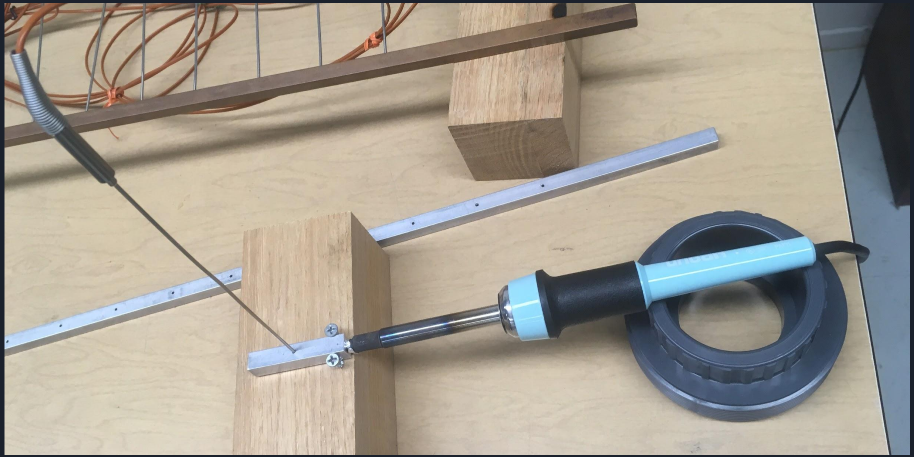
- Motivation
- Background
- Methods
- Results
- Limitations & Future Directions

Motivation

- Understanding data
- Common ODE Models
    - Logistic
    - Exponential



Motivation



- Heated rod experiment
- Sparse regression (SINDy)

Background - **SINDy**

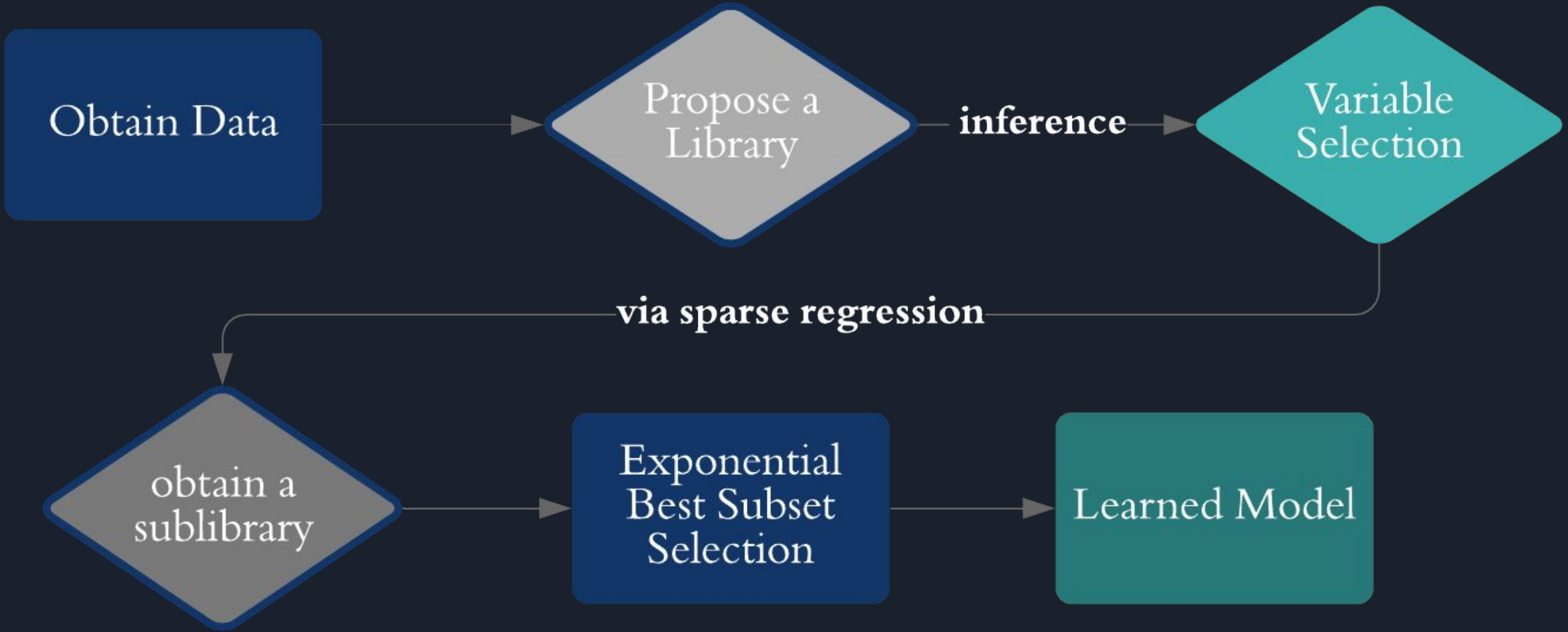
<u>S</u>parse **<u>i</u>**dentification of **<u>n</u>**onlinear **<u>dy</u>**namical systems

A data-driven process to learn an ODE's form -

$$\Theta = [1, y, \ldots y^p, sin(y), cos(y) \ldots]$$

Brunton, S. L., Proctor, J. L., & Kutz, J. N. (2016). Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the National Academy of Sciences*, *113*(15), 3932-3937.

Background - **SINDy**



Background

- Least-Squares Regression
    - Loss Function (Residual Sum of Squares)

$$\hat{\xi} = \underset{\xi}{\operatorname{argmin}} \left(|| \frac{dy}{dt} - \Theta\xi ||_2^2 \right)$$

- Sparse Regression
    - Loss Function + Penalty for Large Coefficients
    - Prevent Overfitting

$$\hat{\xi} = \{\text{Loss}\} + \lambda\{\text{penalty}\}$$

Background

- Ridge Regression
  - L2 Penalty

$$\hat{\xi} = \underset{\xi}{\operatorname{argmin}} \left(|| \frac{dy}{dt} - \Theta\xi||_2^2 + \lambda||\xi||_2^2 \right)$$

- LASSO
  - L1 Penalty

$$\hat{\xi} = \underset{\xi}{\operatorname{argmin}} \left(|| \frac{dy}{dt} - \Theta\xi||_2^2 + \lambda||\xi|| \right)$$

Background

- Best subset selection

$$\text{AIC} = -\frac{2}{N}\log \text{lik} + 2\frac{d}{N}$$

$$\text{BIC} = -2\log \text{lik} + d\log N$$

We are not aware of any study that has performed a full analysis of how LASSO performs when integrated with **SINDy** (as compared to ridge regression and the greedy algorithm).

Methods

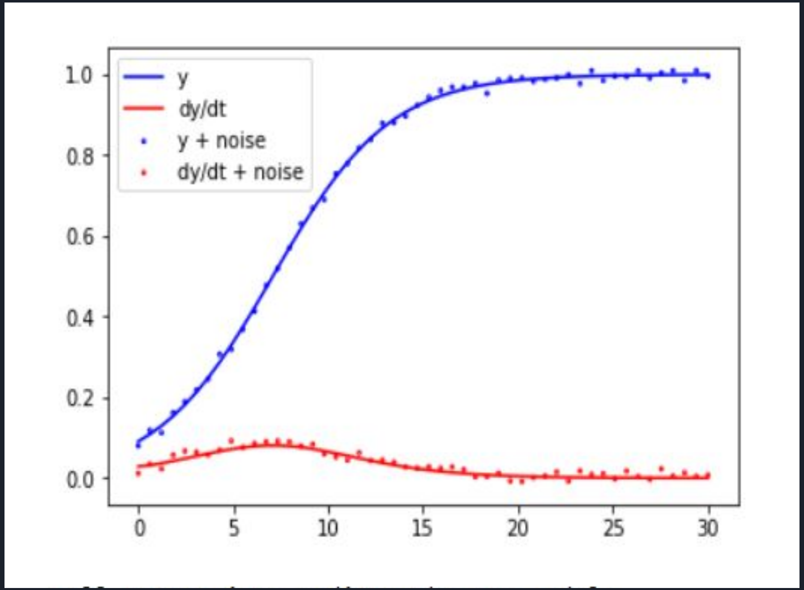
- Simulate data to test SINDy's performance when underlying truths are known
- Assume logistic growth model

$$y = \frac{e^{kt}}{A+e^{kt}}$$

$$\frac{dy}{dt} = ky(1 - \frac{y}{k})$$

- Small amount of gaussian noise

$$\text{Data} = y + \text{Noise}$$



Methods

- We attempt to replicate published methodology using ridge regression with best subsets selection

- We perform all regression in Python using Scikit Learn
    - Optimal hyperparameter and tolerance threshold for ridge regression chosen through 5 fold cross-validation

- After finishing sparse regression, best subsets selection is performed on the selected library terms using AIC/BIC

https://github.com/Xieyangxinyu/SINDy

Methods

- Note that the information criterions have the same general form as the sparse regression algorithms - a loss function with a penalty term

$$\{\text{Loss}\} + \{\text{Penalty}\}$$

$$\text{AIC} = -\frac{2}{N}\log\text{lik} + 2\frac{d}{N}$$

$$\text{BIC} = -2\log\text{lik} + d\log N$$

$$\hat{\xi} = \underset{\xi}{\text{argmin}}\left(||\frac{dy}{dt} - \Theta\xi||_2^2 + \lambda||\xi||\right)$$

$$\hat{\xi} = \underset{\xi}{\text{argmin}}\left(||\frac{dy}{dt} - \Theta\xi||_2^2 + \lambda||\xi||_2^2\right)$$

Methods

Relaxed Lasso

- Use cross-validation to estimate the initial penalty parameter for the lasso
- Apply a second penalty parameter to the selected set of predictor
- Since the variables in the second step have less “competition” from noise variables, cross-validation will tend to pick a smaller value for λ, and hence their coefficients will be shrunken less than those in the initial estimate.

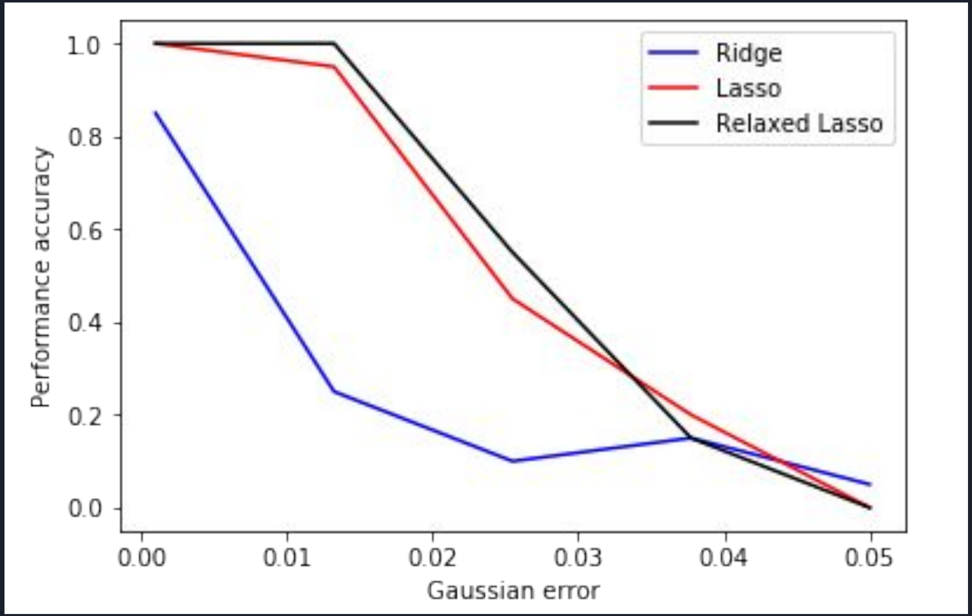
Results

Θ	Ridge CV	Lasso CV	Elastic Net CV	Relaxed Lasso
$u^0, u^1, u^2, u^3, u^4, e^u$	2.86 s	195 ms	221 ms	322 ms
$u^0, u^1, u^2, u^3, u^4, u^5, u^6, u^7$	2.86 s	151 ms	176 ms	306 ms

Results

$$u^0, u^1, u^2, u^3, u^4, u^5, u^6, u^7$$

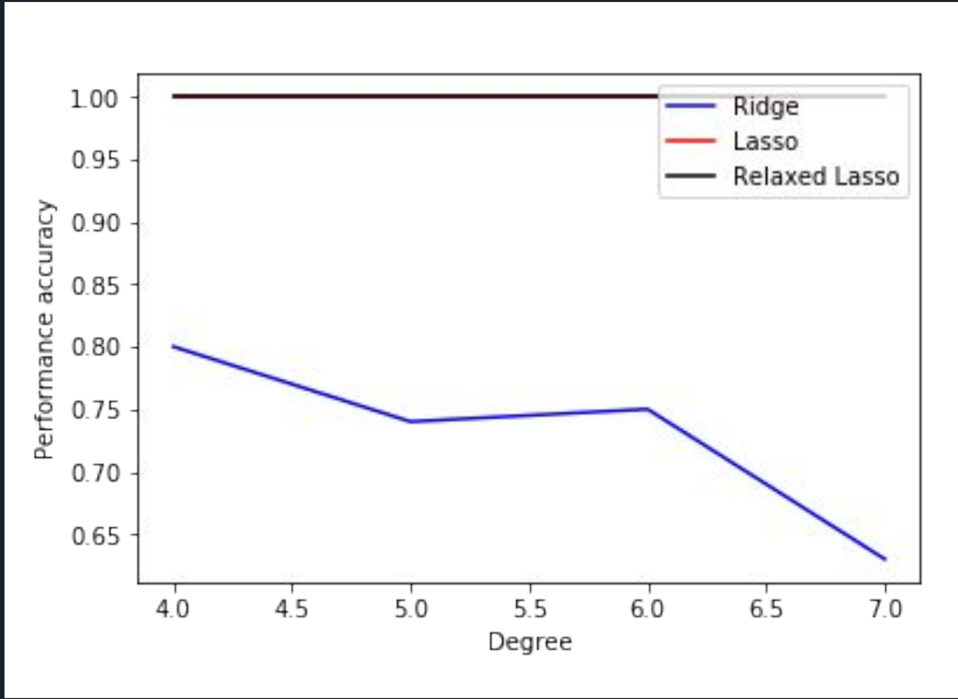
Performance accuracy with increase in the deviance of the Gaussian error



Results

$$u^0, u^1, u^2, u^3, u^4, u^5, u^6, u^7$$

- Relaxed Lasso remains robust throughout as we expand our library from degree 4 to degree 7
- Ridge gets worse

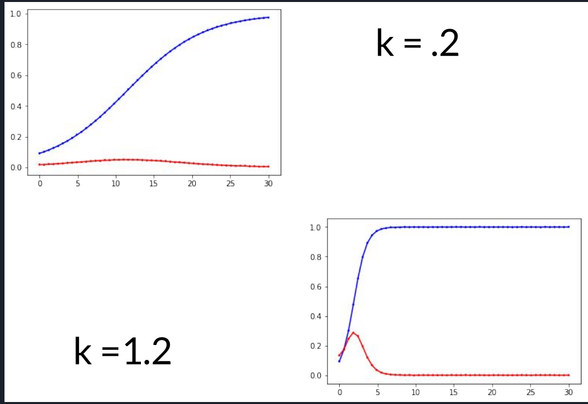


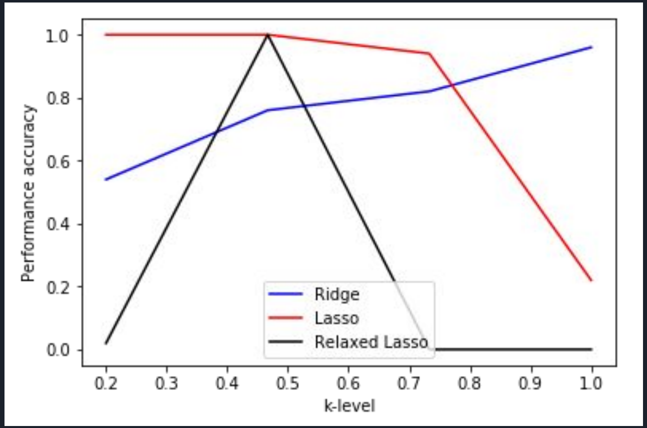
Results

$$u^0, u^1, u^2, u^3, u^4, u^5, u^6, u^7$$

- k represents the range of the data collected
- Suppose we only collect a fixed range of data, the performance of the SINDy model is dependent on the true value of k

$$y = \frac{e^{kt}}{A+e^{kt}}$$

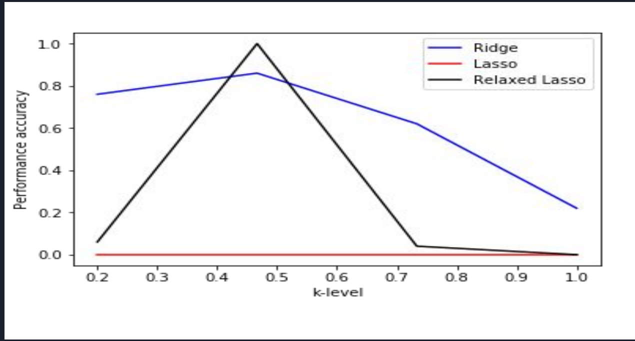


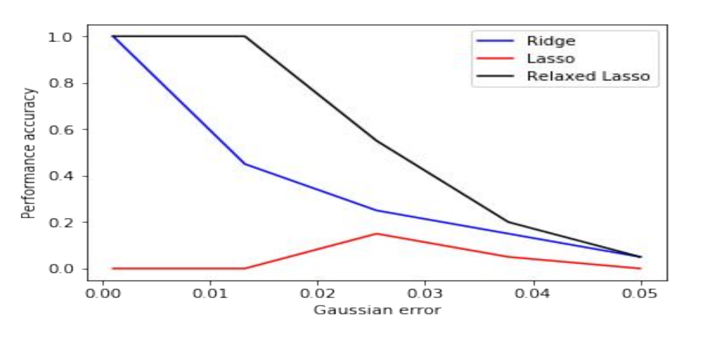


Limitations

- LASSO performs well on high degree polynomial terms but poorly for small order terms. Ridge regression performs well on small order terms but poorly on high degree polynomial terms.
- LASSO performs poorly for exponential terms. Ridge regression performs well, but not as well as relaxed LASSO.

$$u^0, u^1, u^2, u^3, u^4, e^u$$





Limitations

- PCA was surprisingly uninformative
  - One principal component, comprising all non-constant terms in the library, accounted for 98 percent of variation

Alternative Loss and Penalty Functions

Squared Loss:

$$L(y, \hat{f}(X)) = (y - \hat{f}(X))^2$$

Absolute Loss:

$$L(y, \hat{f}(X)) = |y - \hat{f}(X)|$$

Deviance:

$$\begin{aligned} L(G, \hat{p}(X)) &= -2 \sum_{k=1}^{K} I(G = k) \log \hat{p_k}(X) \\ &= -2 \log \hat{p_G}(X) \end{aligned}$$

Hinge Loss:

$$L(y, \hat{f}(X)) = \max\left(0, 1 - y \times \hat{f}(X)\right)$$

Elastic Net Penalty:

$$\min_{\omega \in R^p} \left(\Sigma_{i=1}^{n} l(y_i, \omega^T \times x_i) + \lambda \left[\alpha ||\omega||_1 + \frac{1-\alpha}{2} ||\omega||_2^2 \right] \right)$$

Number of Beta's Penalties

$$\min_{\omega \in R^p} \frac{1}{2} ||y - X\omega||^2 + \lambda_0 ||\omega||_0$$

Conclusion

SINDy is useful for inferring ODE form from data

- Best result: LASSO with cross-validation
- Relaxed LASSO has similar results
- Ridge regression unsuccessful for some libraries

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Questions?