DeepMoD

Model discovery with neural networks

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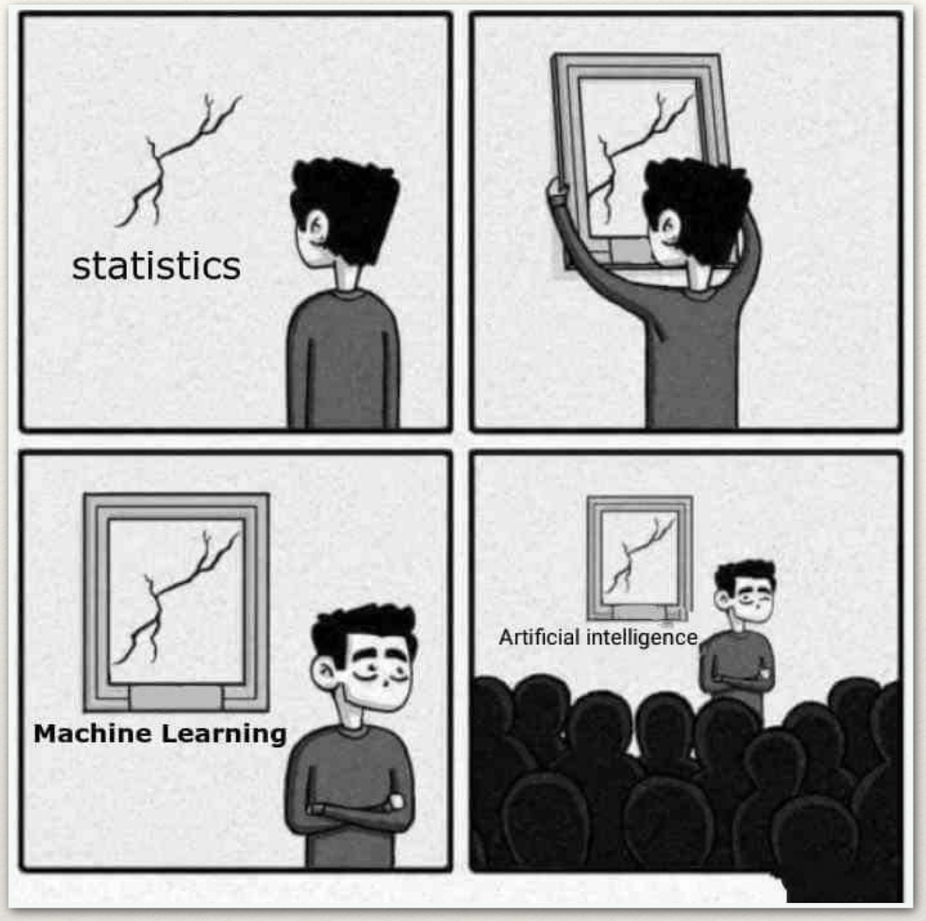
@RemyKusters

AI, ML and statistics



@sandserif

Main criticisms …

ML provides uninterpretable solutions

Statistical ML vs. Symbolic ML

Goal:

Develop tools to discover **interpretable** models for quantitative science

Approach:

Combine the **statistical power of neural networks** with the **symbolic power of regression**

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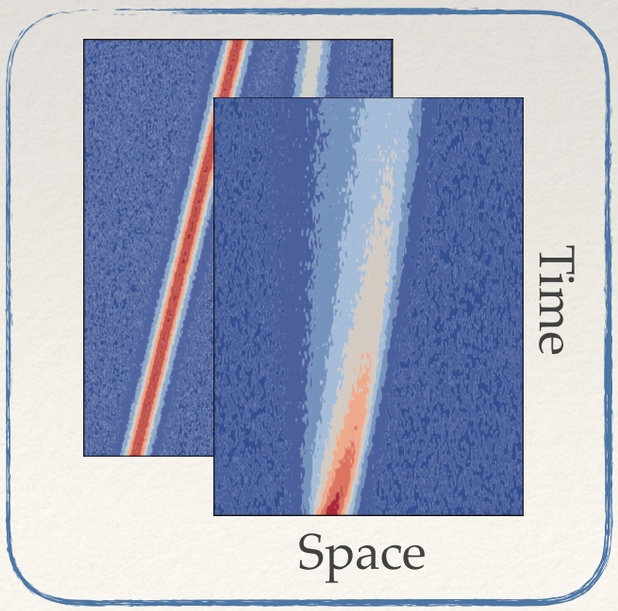
Noisy Data



Differential equation

$$u_t(x,t) = \mathcal{F}(u, u_x, uu_x, u_{xx}, ...)$$

Underlying distribution

$$P(x,t)$$

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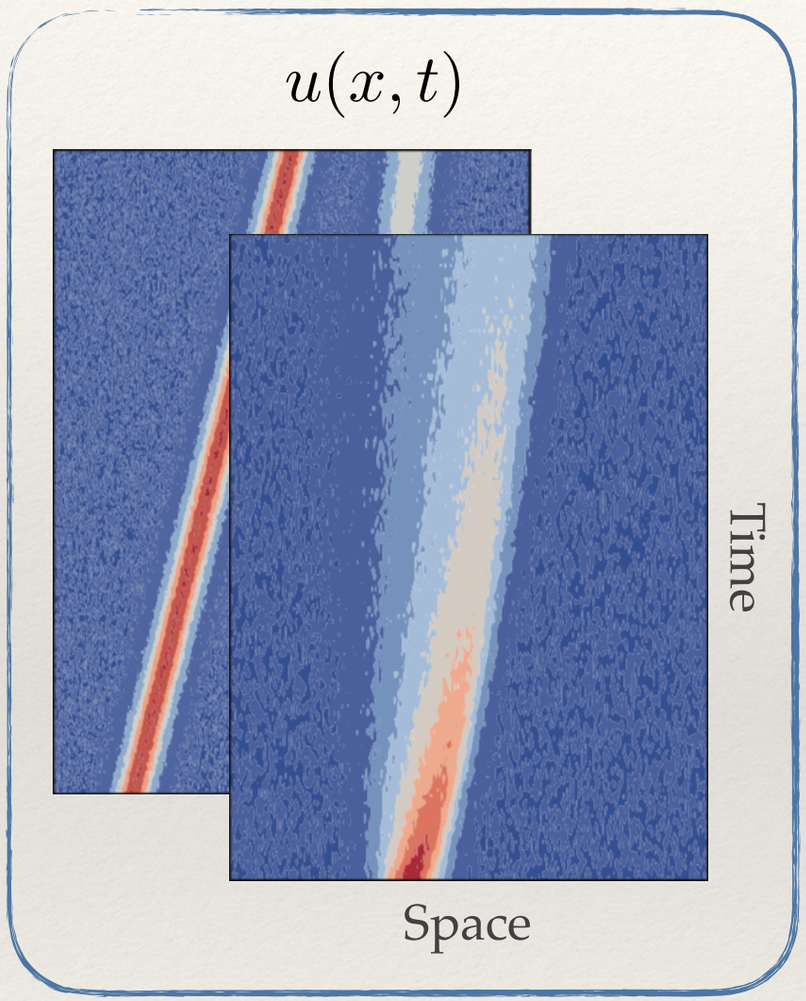
Noisy Data



Analytic solution

$$u_t(x,t) = \mathcal{F}(u, u_x, uu_x, u_{xx}, ...)$$

Code available:
github.com/PhIMaL

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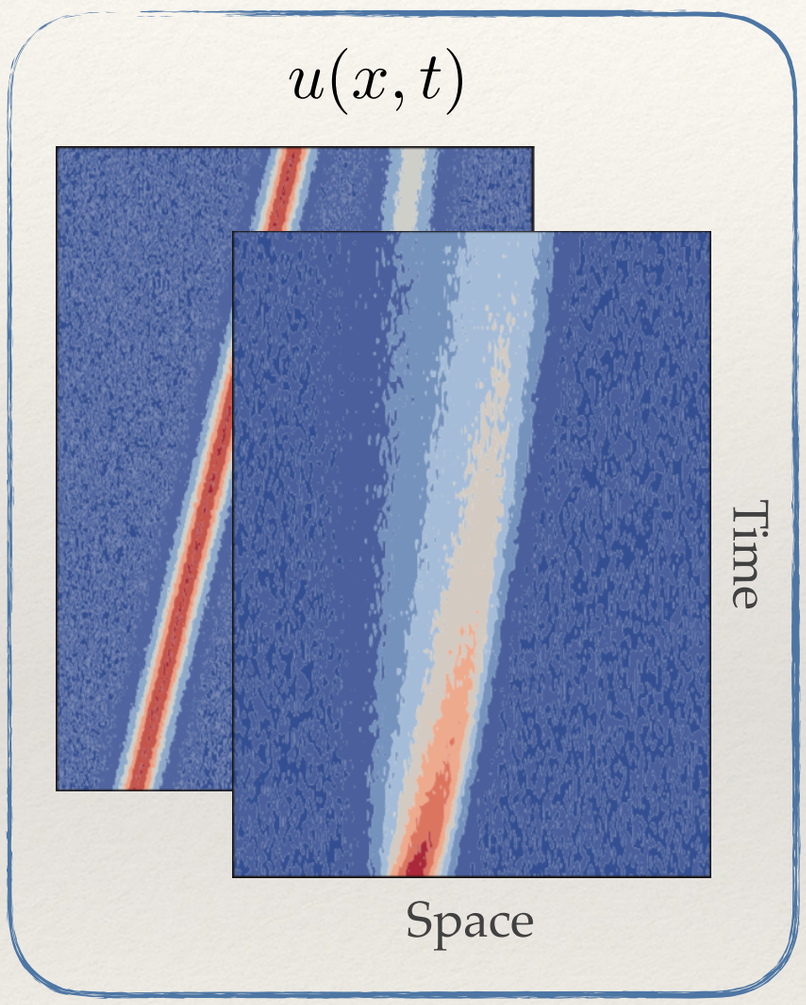

Solution

$$u_t(x,t) = \Theta\vec{\xi}$$

$$\begin{bmatrix} \\ \\ \end{bmatrix} = \begin{bmatrix} u \\ u_x \\ uu_x \\ \vdots \\ u^2u_{xx} \end{bmatrix} \begin{bmatrix} \\ \\ \end{bmatrix}$$

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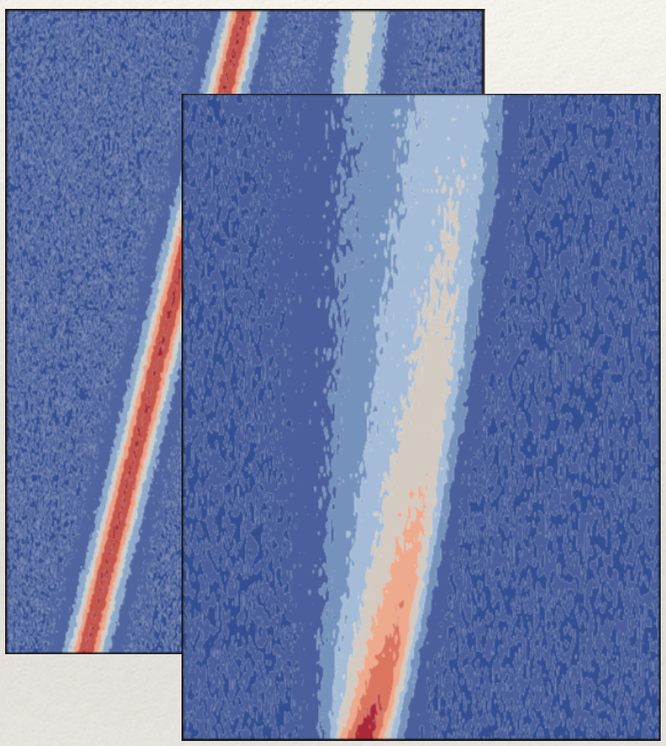
Noisy Data

$u(x,t)$



Regression

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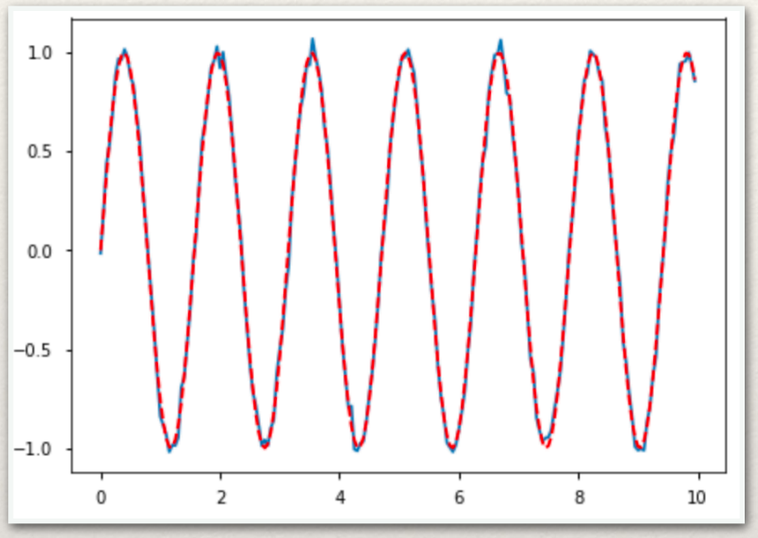
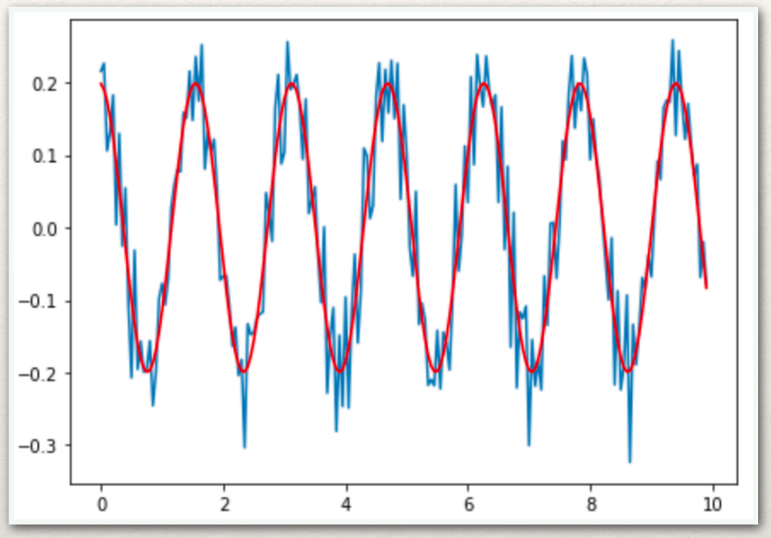
Why does it fail with noise?

5% white noise …

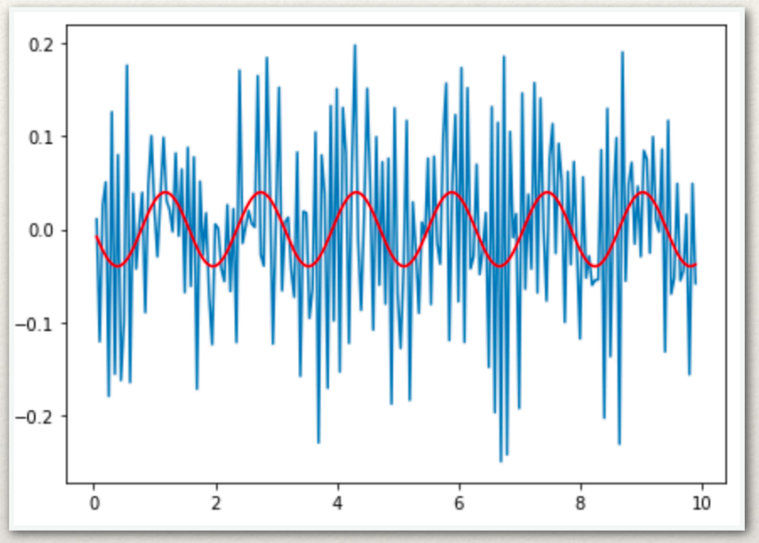
$u(x)$



$u_x(x)$



$u_{xx}(x)$

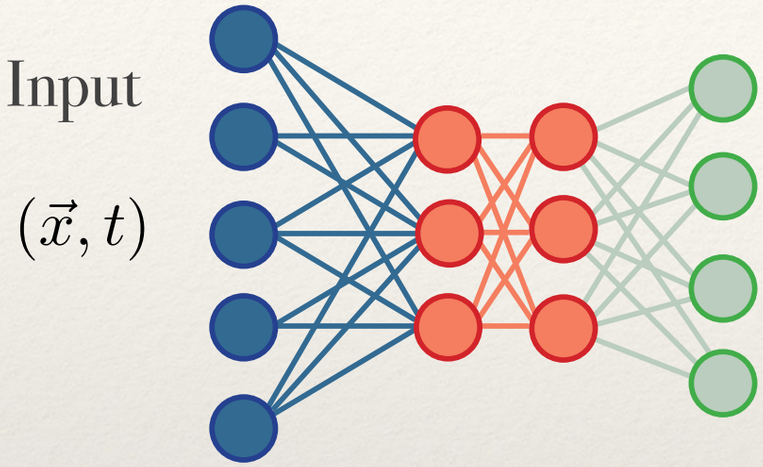


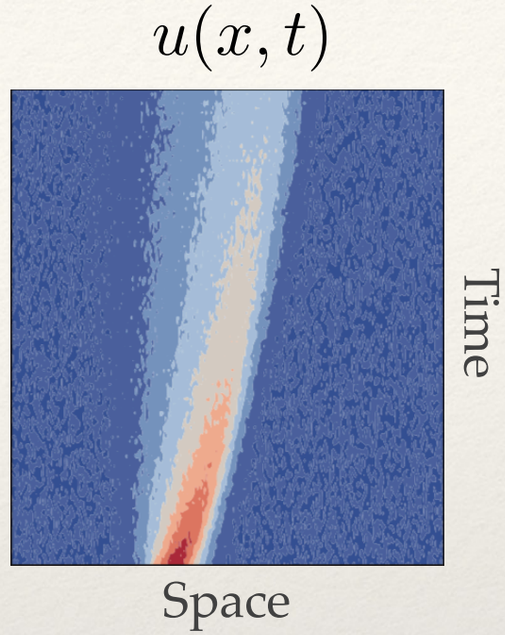
$$\Theta = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ u & u_x & u_x u & u_{xx} & u_{xx} u & u_{xx} u_x & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

Numerically calculating library impossible …

Our approach …

The Neural Network





Construct the library w.r.t. **the inferred solution**

$$\Theta = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ \hat{u} & \hat{u}_x & \hat{u}_x\hat{u} & \hat{u}_{xx} & \hat{u}_{xx}\hat{u} & \hat{u}_{xx}\hat{u}_x & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

Include the **regression task** within the neural network

How do we train a neural network

Optimise loss function:

$$\mathcal{L} = \mathcal{L}_{MSE} + \mathcal{L}_{Reg} + \mathcal{L}_{L_1}$$

Approximate the data as good as possible ...

Learn the mapping
$(\vec{x}, t) \rightarrow \vec{u}$

$$\mathcal{L}_{MSE} = \frac{1}{N} \sum_{i=1}^{N} |u(\{x,t\}_i) - \hat{u}_i|^2$$

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Discover the differential equation

Regression
(Seek the PDE)

$$\mathcal{L}_{Reg} = \frac{1}{N} \sum_{i=1}^{N} |\Theta_{ij}\xi_j - \partial_t \hat{u}_i|^2$$

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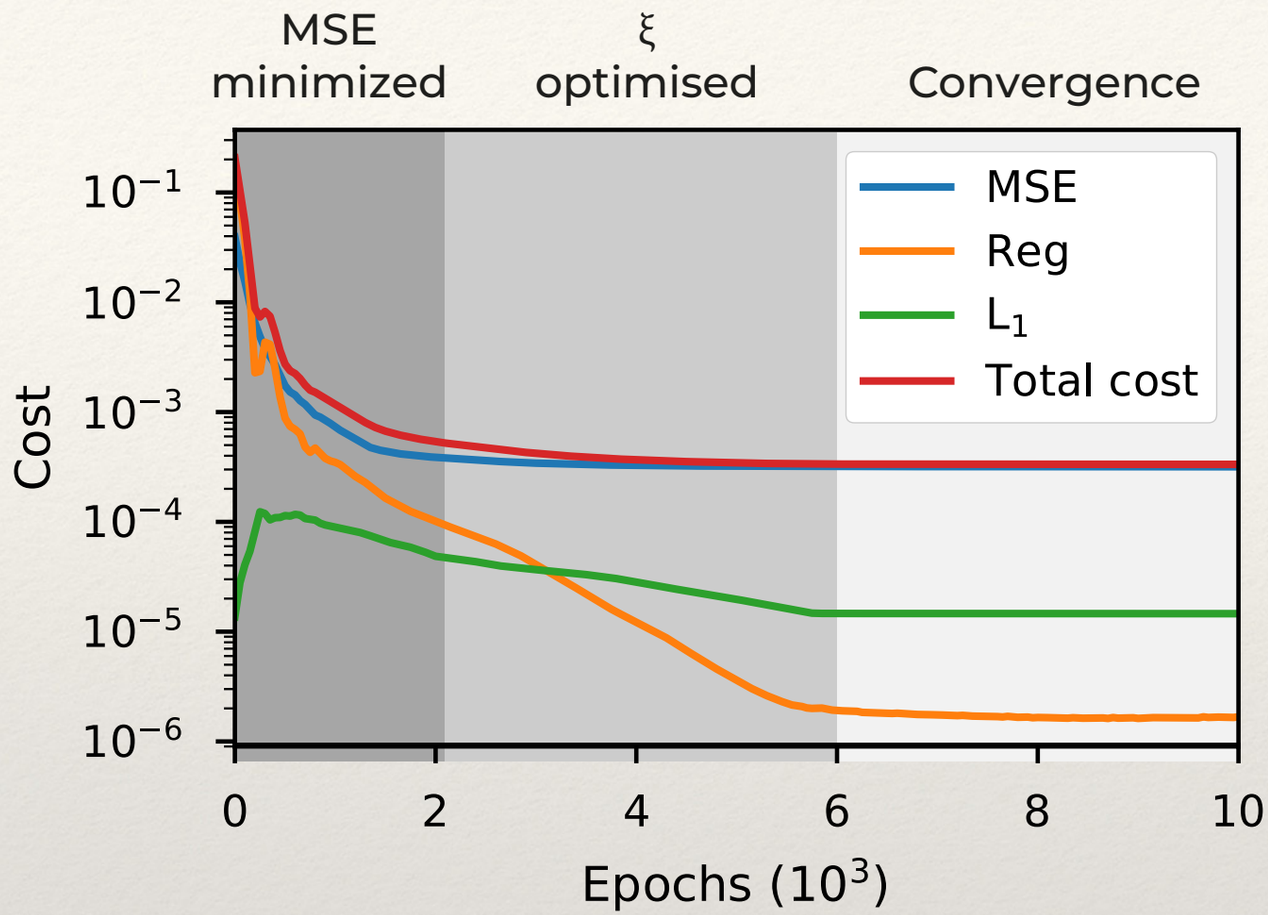
Promoting sparsity

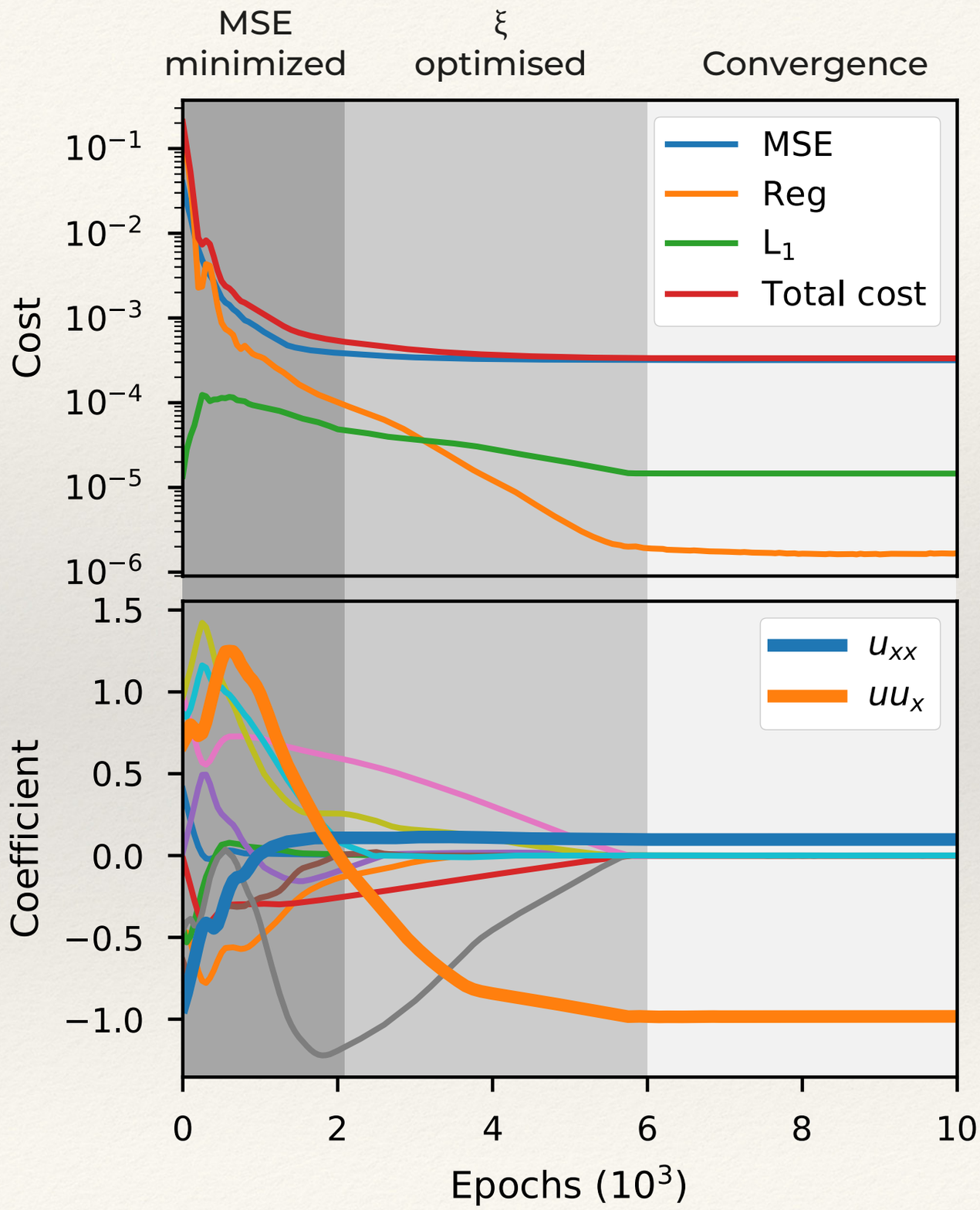
L1 Penalty

$$\mathcal{L}_{L_1} = \lambda \sum_{i=2}^{M} |\xi^i|$$

Training the neural network



Training the coefficient vector



$$u_t(x,t) = \Theta\vec{\xi}$$

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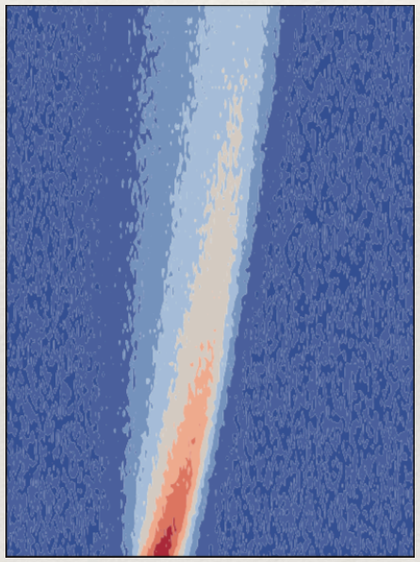
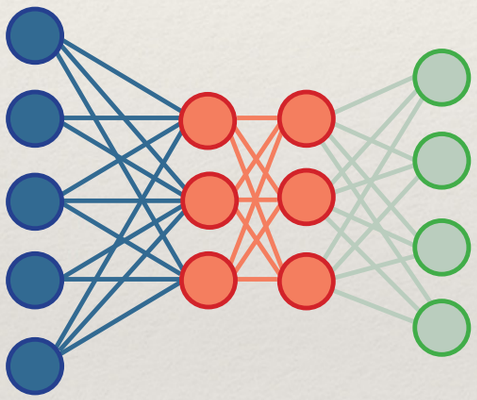
$u(x,t)$



Neural network

$(\vec{x},t)$ → $\hat{u}$



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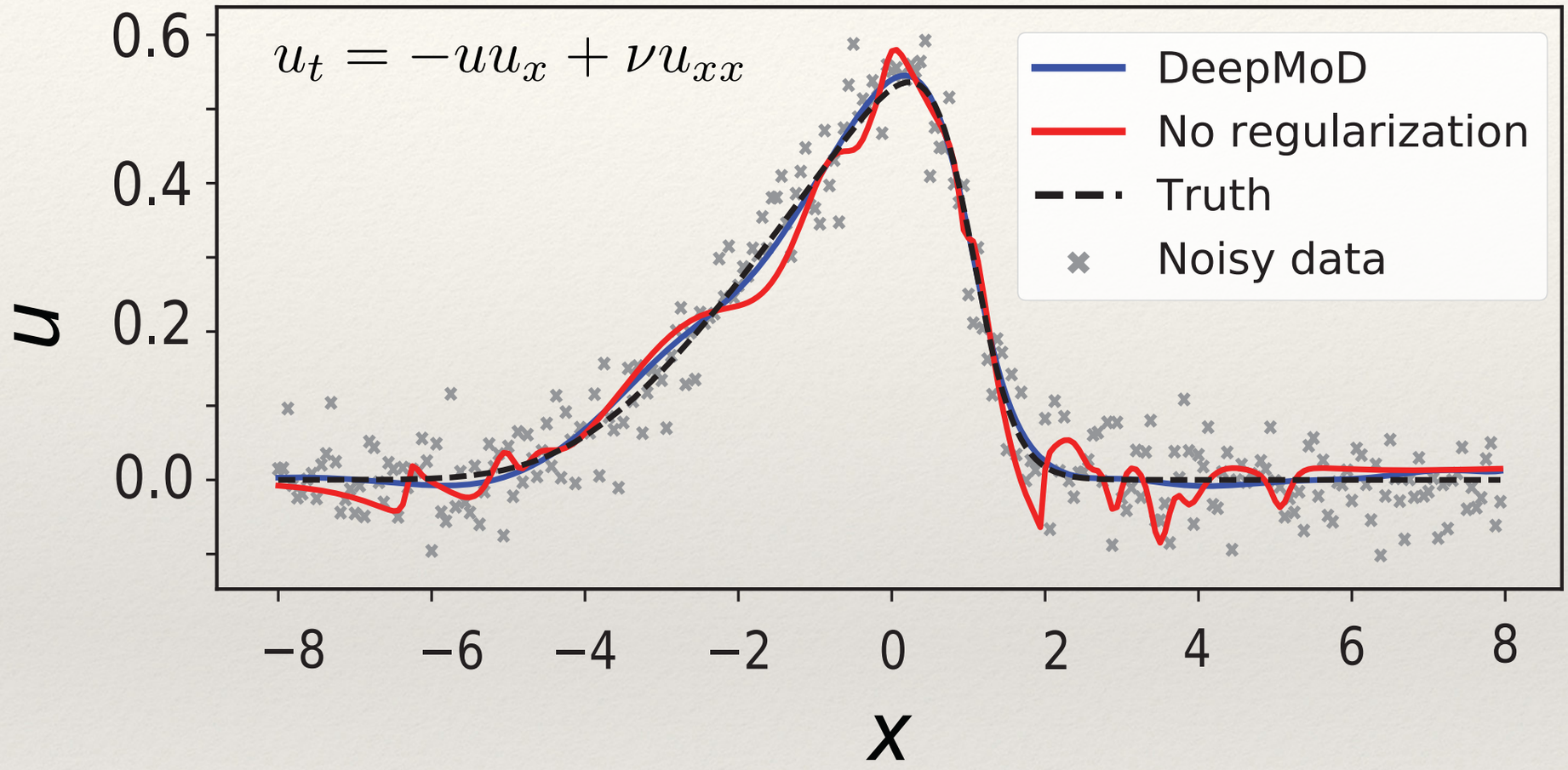
Why regression inside neural network?



Applications in physics

Resilience to Noise/ sampling size

Burgers' equation

$$u_t = -uu_x + \nu u_{xx}$$

Relative error on coefficients

Higher order PDEs

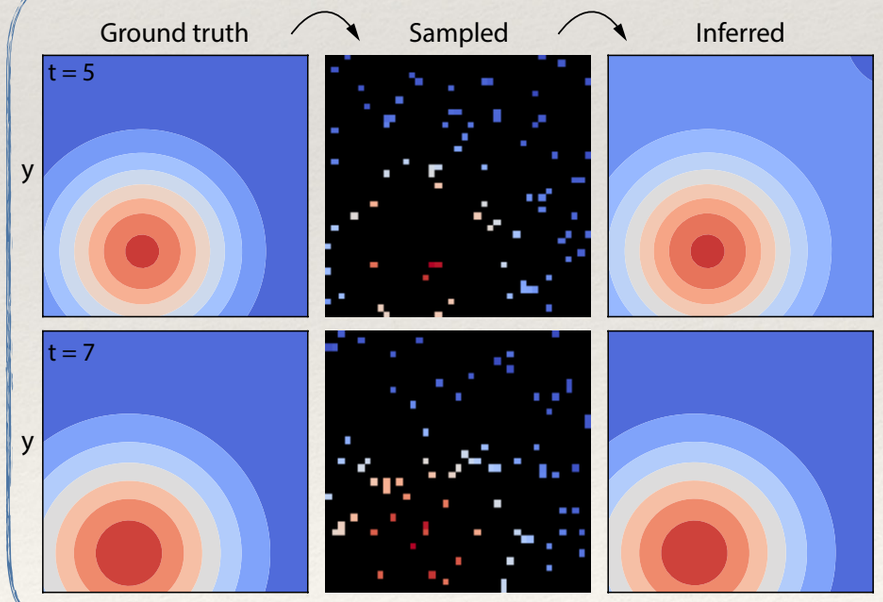
$$u_t = 6uu_x - u_{xxx}$$

Coupled equations

$$u_t = \nabla \cdot (D_i \nabla u - \xi u \nabla w) \quad u \text{ :particle density}$$

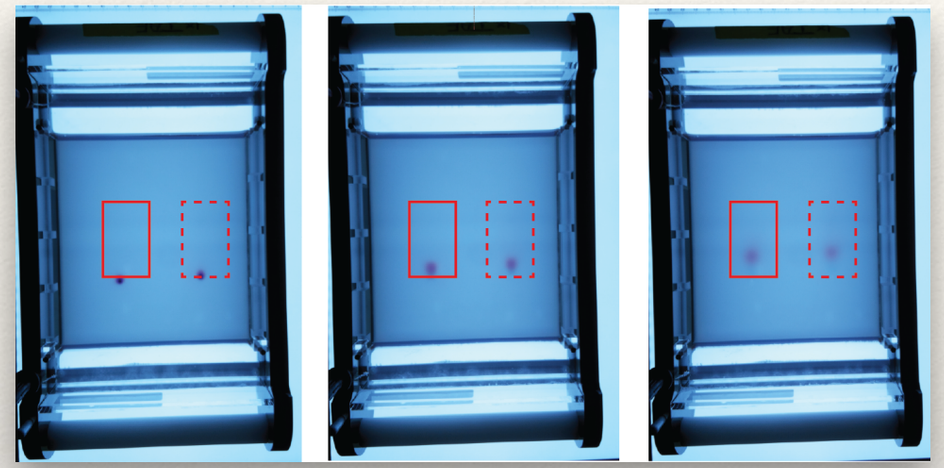
$$w_t = D_w \Delta w - kw + hu \quad w \text{ :attractant density}$$

2D equations

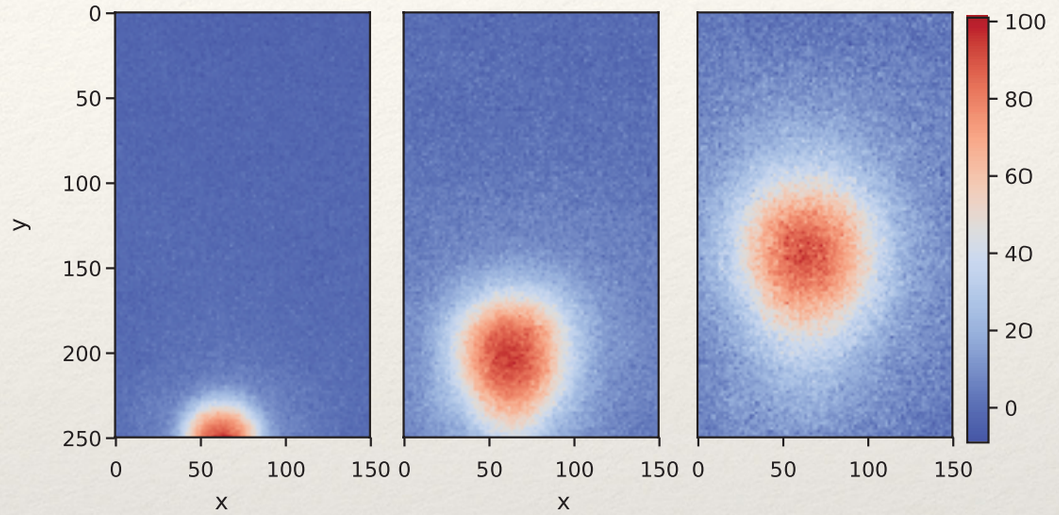


Apply to real data …

Raw images



Density field



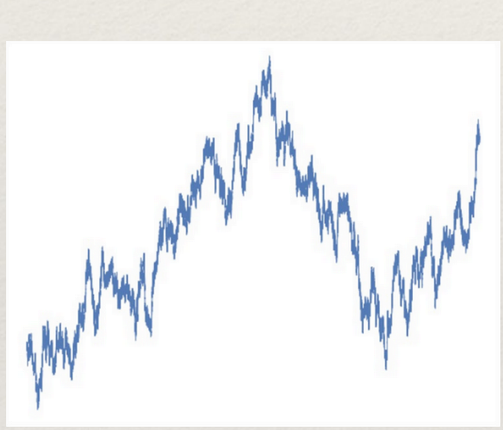
Underlying AD equation

$$u_t = 0.3u_y + 0.01u_{xx} + 0.01u_{yy}$$

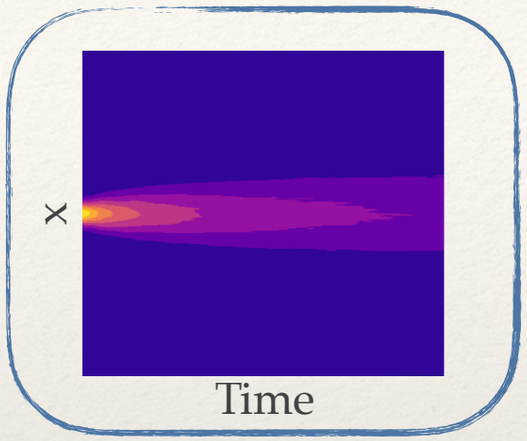
Model discovery from **experimental data**

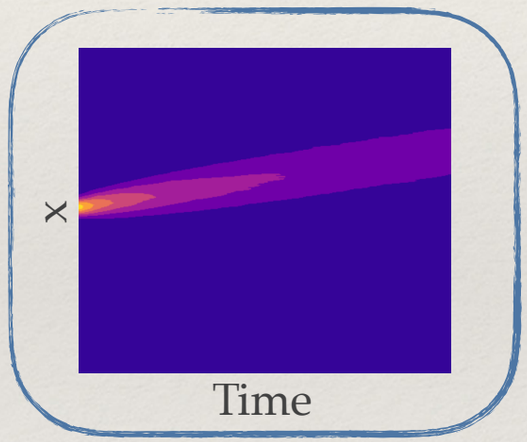
Single Particle Tracking

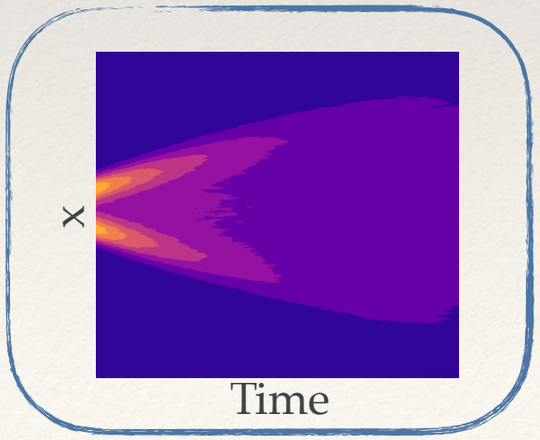
Trajectory



Density estimation







Model discovery

Random walk

$$u_t = Du_{xx}$$

Advected random walk

$$u_t = Du_{xx} + v_d u$$

Persistant random walk

$$u_{tt} + \frac{1}{\tau_c} u_t = \nu^2 u_{xx}$$

Single Particle Tracking

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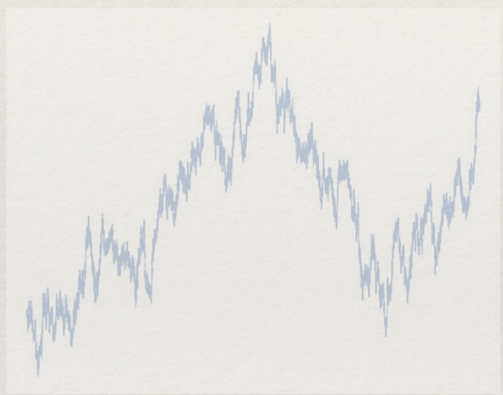
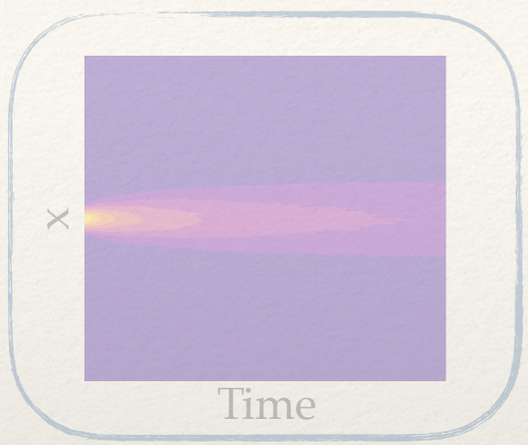
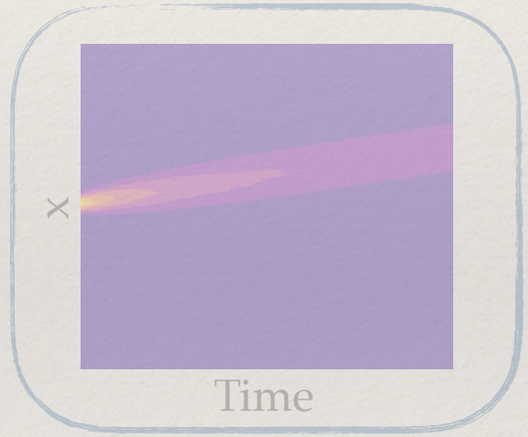
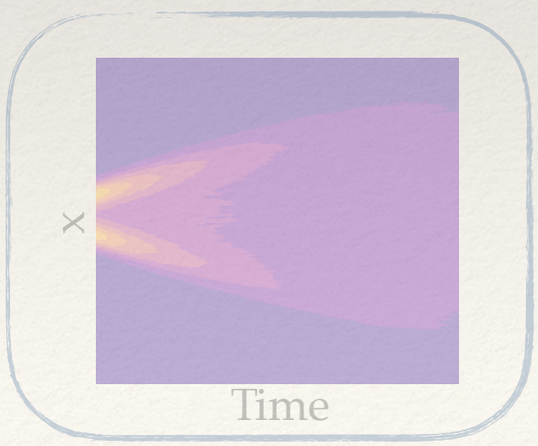


Density estimation







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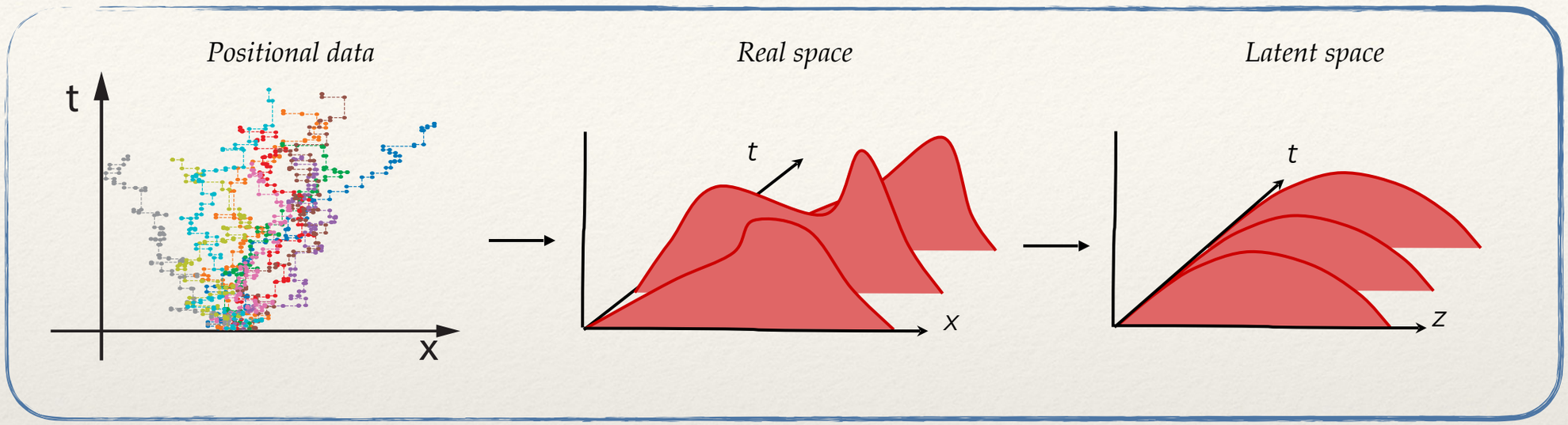
Density estimation: Temporal normalizing flows



Temporal Normalizing Flows (tNFs) extend NFs with a temporal component to estimate a **time-dependent density evolution**

Code available on Github:
https://github.com/PhIMaL

Paper available on arXiv:
1912.09092

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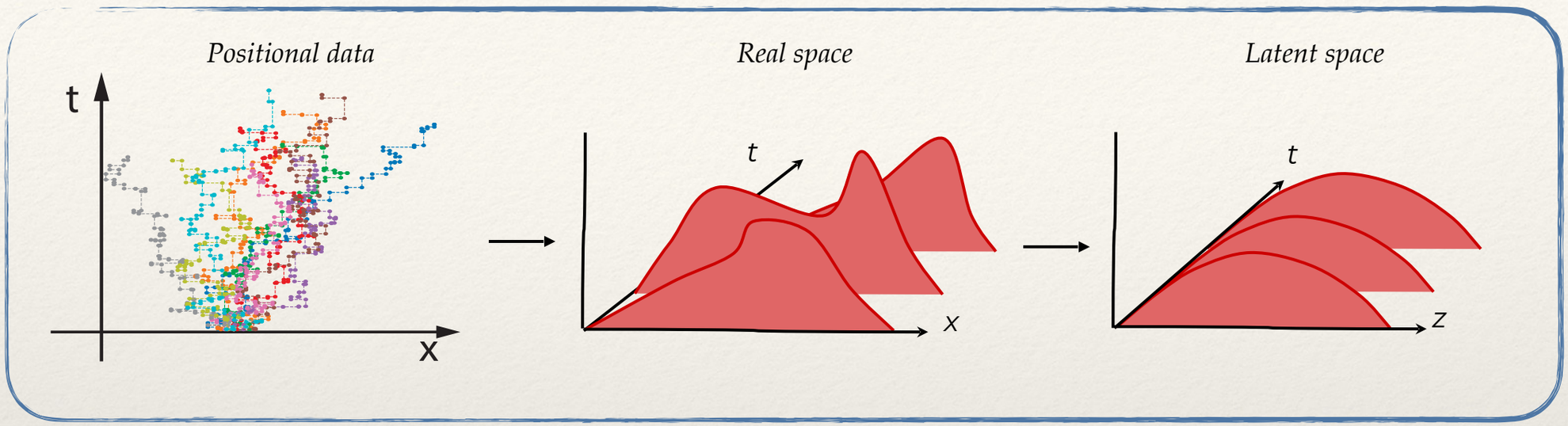

Temporal Normalizing Flows (tNFs) extend NFs with a temporal component to estimate a **time-dependent density evolution**

tNFs allow discovery of PDEs with conservation constraints, e.g. Fokker-Planck, ...

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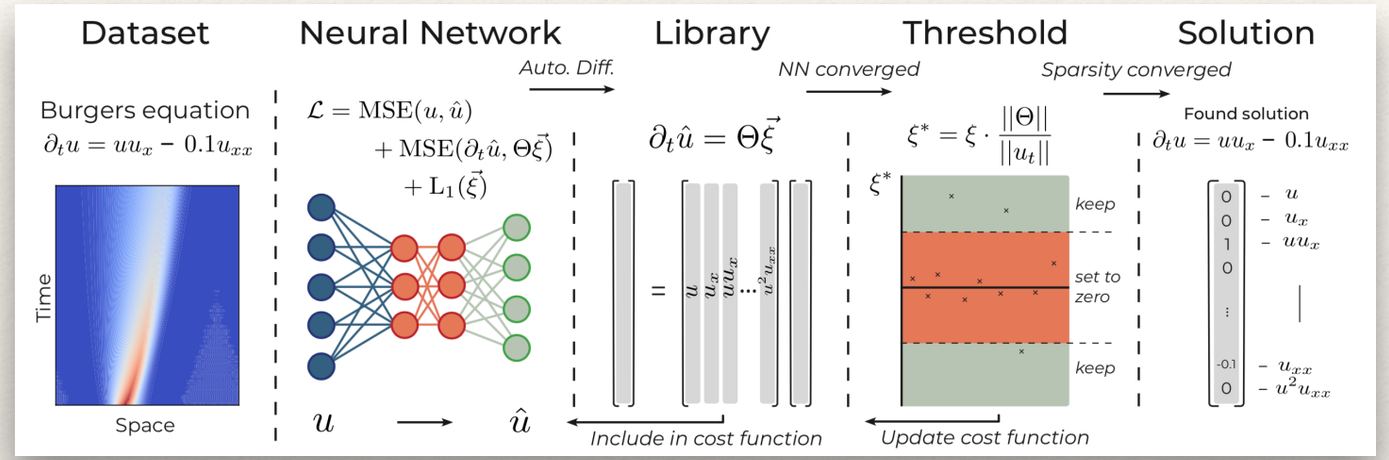

Code available on Github:
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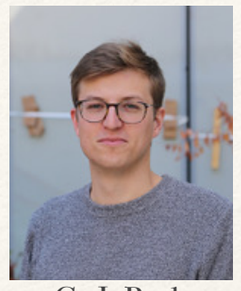
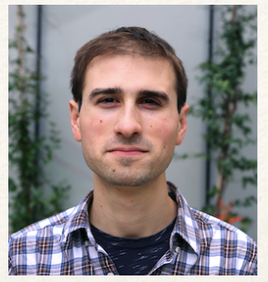
Paper available on arXiv:
1904.08406



G.-J. Both
(PhD)



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C. Le Scao
(Intern)

T. Chrysostomou
(Intern)

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@RemyKusters

TensorFlow

PyTorch

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