Lecture 7. Neural ODES for, and as, dynamical systems

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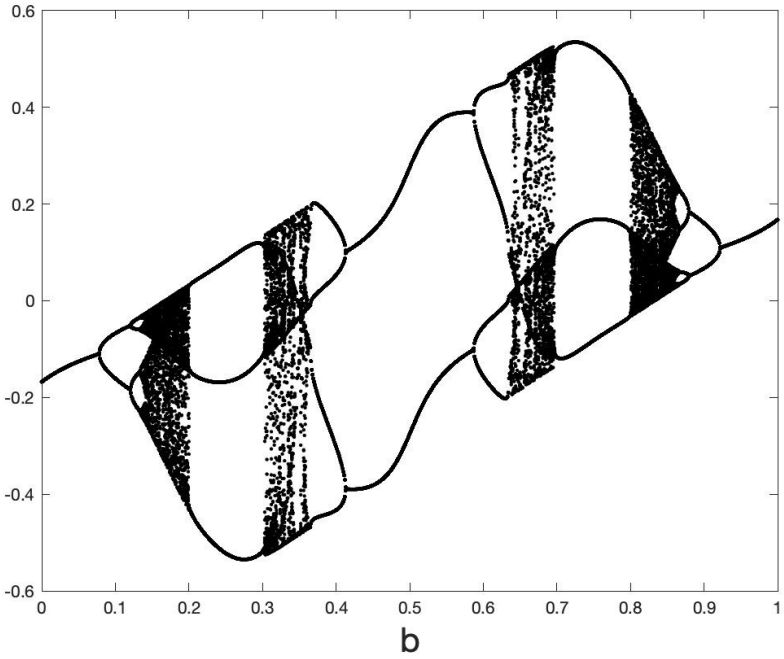
Seattle, June 2025



Some papers/books to look at

- Chen et. al., *Neural Ordinary Differential Equations*
- Matlab and Simulink, *Dynamical System Modelling Using Neural ODE*
- di Bernardo et. al., *Piecewise smooth dynamical systems*
- Brunton, Kutz et. al, *Discovering governing equations from data by sparse identification of nonlinear dynamical systems*
- Ashwin et. al. *RNNS*

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Dynamical systems

Flows:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t, \theta)$$

Maps:

$$\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n, \theta)$$

$x(0), \quad x_0$ Given. Study the evolution from this state

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Dynamical systems link to neural networks in a number of ways

- Solving a dynamical system using a PINN .. See lecture 3
- Constructing a dynamical system operator using a Neural Operator .. See lectures 5 and 6
- Approximating the flow through a NN as a dynamical system (Neural ODE 1) [Chen et. al.]
  and train that dynamical system
- Using a NN to approximate/learn the RHS of a dynamical system by

$$\frac{du}{dt} = f(\mathrm{t}, \mathrm{u}, \theta)$$

where f is the output of a NN and learn the parameters θ from data (Neural ODE 2)

- Take f to be symbolic and learn it from data. SINDy [Brunton et. al.]
- Predict the dynamics of a dynamical system using a LSTM or similar

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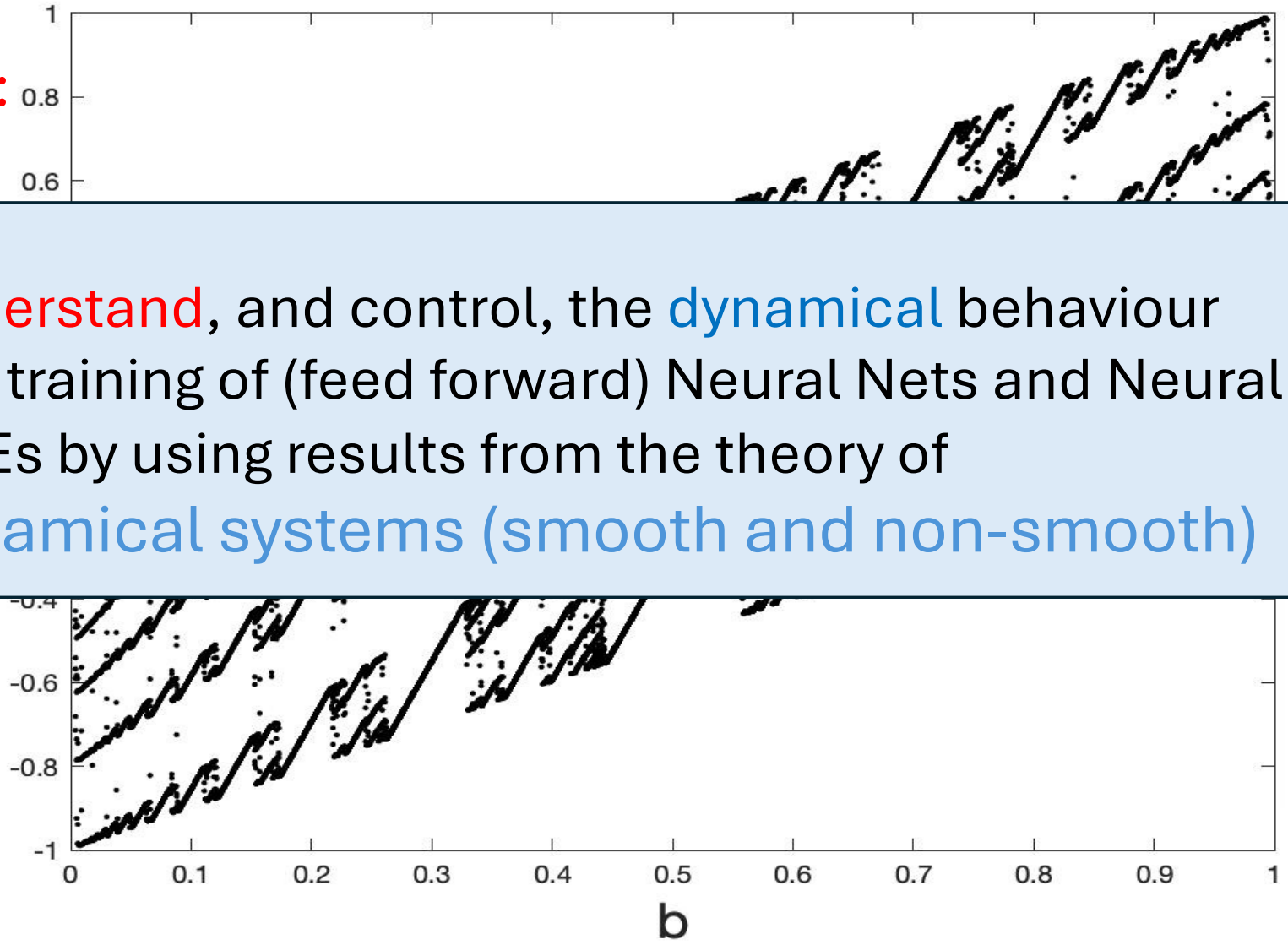
AIM:



Understand, and control, the dynamical behaviour and training of (feed forward) Neural Nets and Neural ODEs by using results from the theory of dynamical systems (smooth and non-smooth)

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Basic properties of smooth dynamical systems e.g. dx/dt = f(t,x)

Evolve from initial state x_0

Transient motion followed (usually) by convergence to an omega-limit set ω

Omega limit sets ω depends on the parameters θ can be:

- Attracting Fixed Points. (FPs)
- Periodic orbits
- Heteroclinic connections
- Quasi-periodic orbits
- Chaotic strange attractors

Varying θ leads to smooth changes of the omega-limit set, and changes/transitions between different types of omega-limit set at bifurcations

[See Ashwin et. el apply this methodology to RNNs,ESNs,ENAs]

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Examples of smooth bifurcations:

Saddle node and tipping points

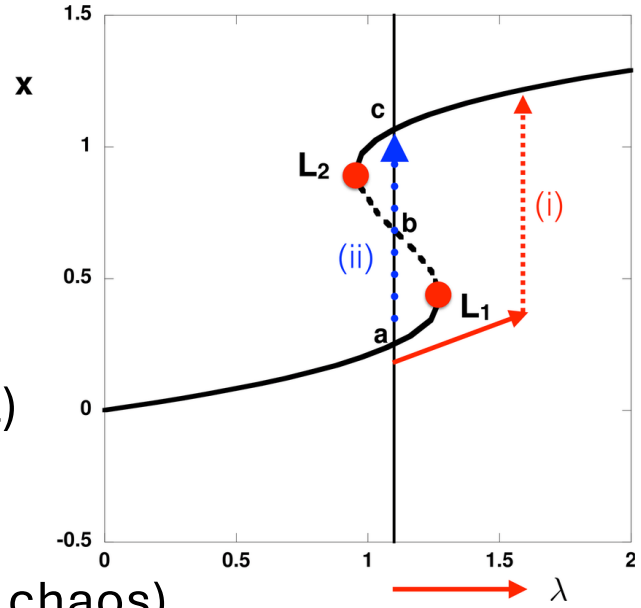
Transcritical and Pitchfork (super and sub critical)

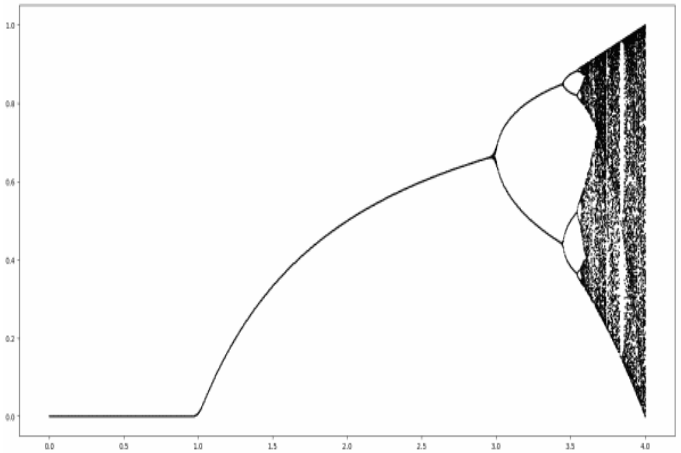
Period-doubling (and period doubling cascade to chaos)

Hopf (super and sub critical)

Cyclic fold

Homoclinic/heteroclinic





NNs as Dynamical Systems

All feed forward NNs and RNNs can be thought of as maps:

Eg.

$$x_{n+1} = \sum_i c_i^n \sigma(A_i^n x^n + b_i^n)$$

Defines a parametrized map

NN: Input x_0 output x_N .

Deep if N >>1. Then we can study the output of the NN as the omega limit set of the map. Training then relates to how the omega limit set depends on the parameters eg. bifurcations etc.

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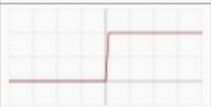
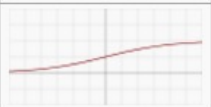
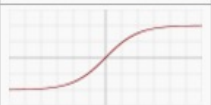
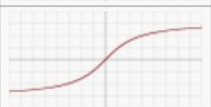
Can be

Smooth

Or

Non-smooth

Depending on the activation function

Name	Plot	Equation	
Identity		$f(x) = x$	
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	Discontinuous
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	Smoothed discontinuous
ArcTan		$f(x) = \tan^{-1}(x)$	
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	Discontinuous derivative
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	Discontinuous derivative
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	
SoftPlus		$f(x) = \log_e(1 + e^x)$	

Lack of smoothness can lead to very rich dynamics

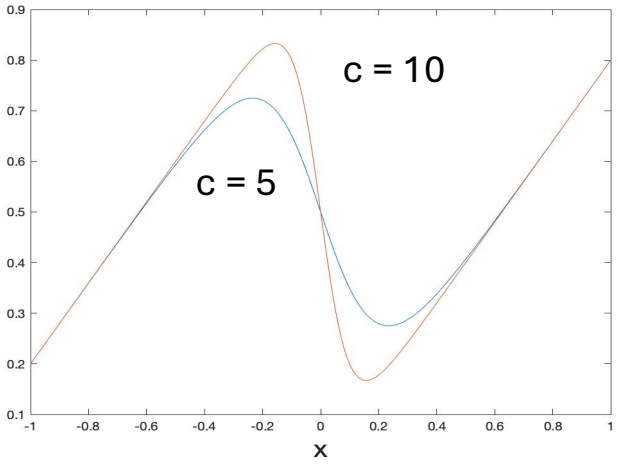
Partly explains the great expressivity of a deep neural network

Case Study : Feed forward NN: One-d smoothed sigmoid map

$$x_{n+1} = a\, x_n - H(x_n) + b, \quad H(x) = 1, x \geq 0, \quad H(x) = 0, x < 0$$

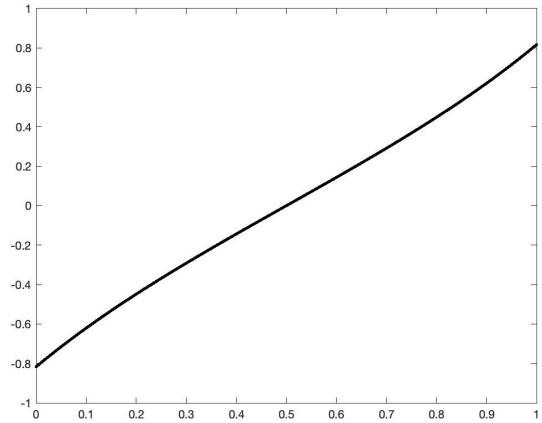
Smoothed to:

$$x_{n+1} = a\, x_n - (1 + \tanh(c\, x_n))/2 + b.$$

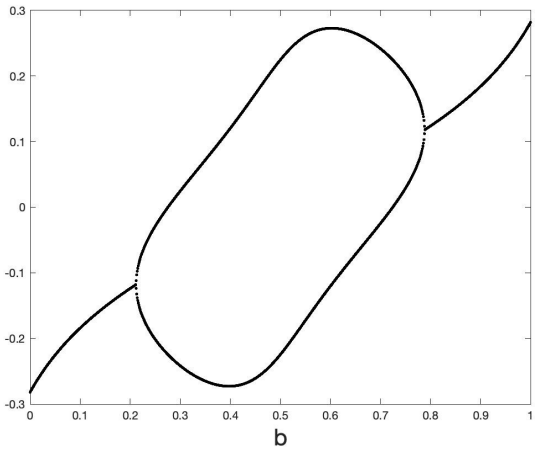


Omega-limit sets as a function of smoothing (when a = 0.8)

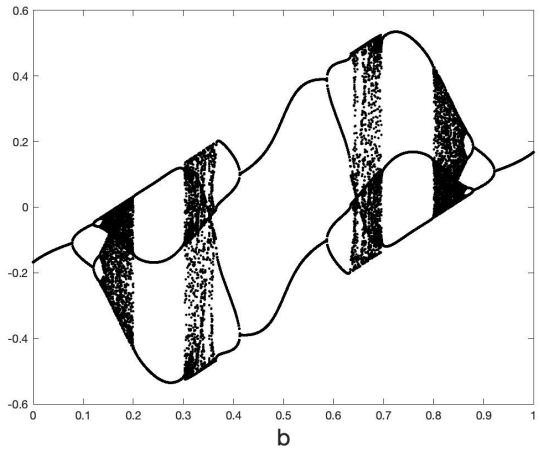
c = 1



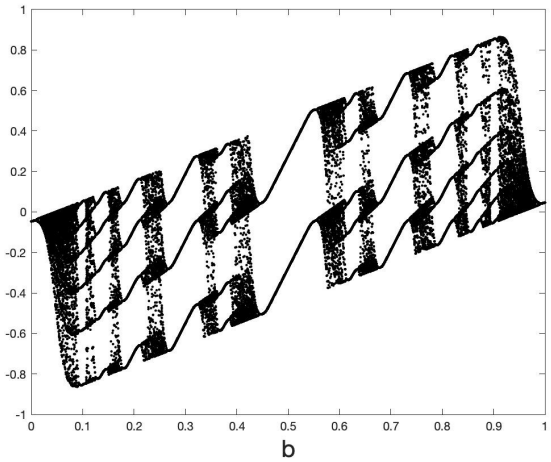
c = 5



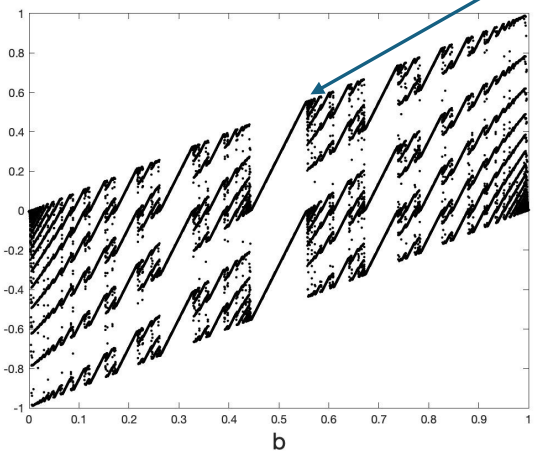
c = 10



c = 50

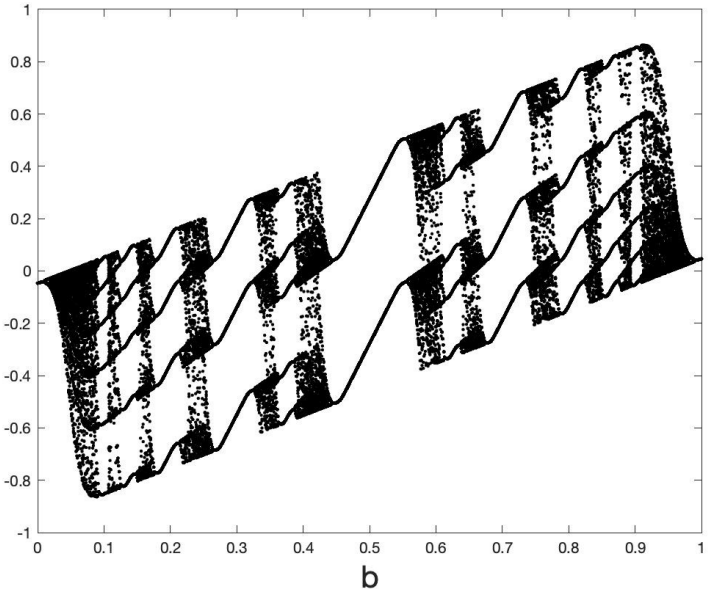


c = 1000



Border collision

Conclusions from the results



- High gradient of the tanh function leads to chaotic behaviour in certain cases. Hard to define a loss function and dependence of the loss function on the input/parameters in this case

Consider $\theta = \{a,b,c\}$ to be trainable parameters

- Only in the case of c = 1 is dependence on the training smooth and predictable using back propagation

- Sensitive parameter dependence can make training difficult close to bifurcation points b^* giving a loss function changing as $1/\sqrt{b-b^*}$ in the smoothed case and period adding at the border collision.

- But allows great expressivity

Neural ODES [Chen et. al] : The ResNET architecture as a flow

$$x_{n+1} = x_n + \Delta t \sum_i c_i^n \sigma(A_i^n x^n + b_i^n)$$

Let $t = n\,\Delta t$

$$\frac{x_{n+1} - x_n}{\Delta t} = \sum_i c_i(t)\ \sigma(A_i(t)x^n + b_i(t))$$

Let $\Delta t \ \rightarrow 0$

$$\frac{dx}{dt} = \sum_i c_i(t)\ \sigma(A_i(t)x^n + b_i(t))$$

Neural ODE. Input: x(0). Output: x(T), $T = n\,\Delta t$

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- Idea [Chen et. al.]:
- Replace the NN by solving the Neural ODE using an ODE solver eg. RK4, Adam
- Training now becomes a question of finding the functions A(t), b(t), c(t)
- Advantages in memory efficiency and back propagation
- This a problem in optimal control theory

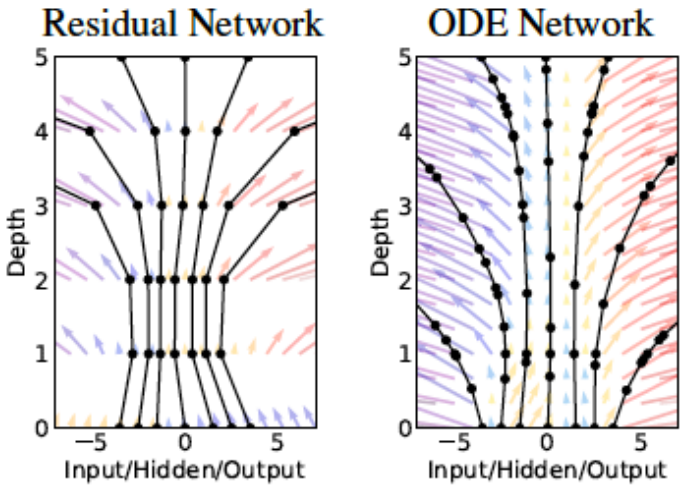

Figure 1: *Left:* A Residual network defines a discrete sequence of finite transformations. *Right:* A ODE network defines a vector field, which continuously transforms the state. *Both:* Circles represent evaluation locations.

Training such a ‘Neural ODE’. [Chen et. al 19], [Pontryagin 62]

Consider the parametrized Neural ODE

$$\frac{d\mathbf{h}}{dt} = f(\mathbf{h}(t), t, \theta), \quad \mathbf{h}(0) \to \mathbf{h}(T).$$

Compute solution using an ODE solver

Loss function L(.)

$$L(\mathbf{z}(T)) = L\left(\mathbf{z}(0) + \int_0^T f(\mathbf{z}(t), t, \theta)\, dt\right)$$

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To train the neural net to optimize L we need to find how it changes with θ

Results from classical control theory (and data assimilation) allow us to do this

Step 1

Define adjoint $\mathbf{a}(t) = \partial L / \partial \mathbf{z}(t)$ then

$$\frac{d\mathbf{a}}{dt} = -\mathbf{a}^T \, \partial f / \partial \mathbf{z}$$

Compute a(t) using an ODE solver ‘backwards’ starting from z(T)

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Step 2

Compute the gradient of L by solving a third ODE

$$\frac{dL}{d\theta} = -\int_T^0 \mathbf{a}(t)^T \frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \theta} \, dt$$

Can then train θ to optimize L using gradient descent

[Chen et. al.] implement this using an adaptive Adam solver.

What can a Neural ODE be trained to do? Homeomorphism Theorem

Classical Neural ODEs take the form of

$dh/dt = f(h,t,\theta)$ where f is a Lipschitz function constant L

Want to train this so that we have the map. F: h(0) $\longrightarrow$ h(T)

Theorem *If f is Lipschitz than F is continuous*

Proof Let F: u(0) $\longrightarrow$ u(T) and F: v(0) $\longrightarrow$ v(T), z(t) = u(t) – v(t)

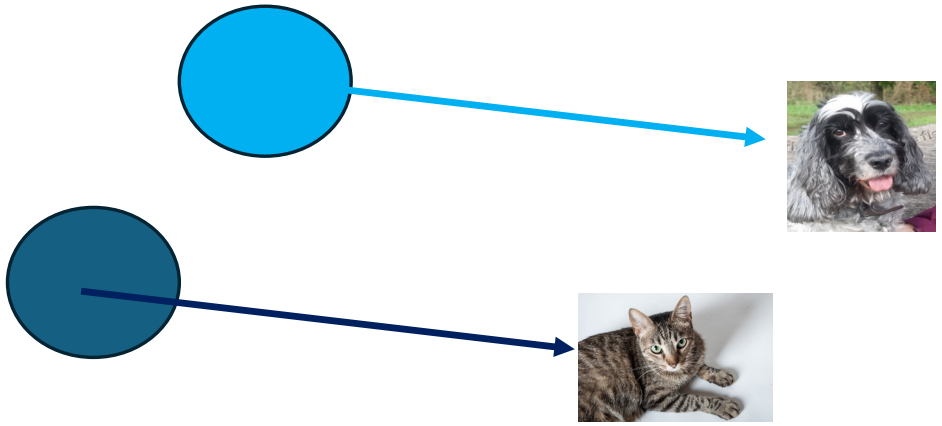
dz/dt = f(u,t) – f(v,t) < |f(u,t) – f(v,t)| < L |u – v|. Therefore

$$|u(T) - v(T)| < e^{Lt} |u(0) - v(0)|$$

Conclusion:

Topology of the input data is the topology of the output data

Example: Want to train a Neural ODE to separate data eg. dogs and cats. [+Davide Murari]



Can resolve this topology with a Neural ODE

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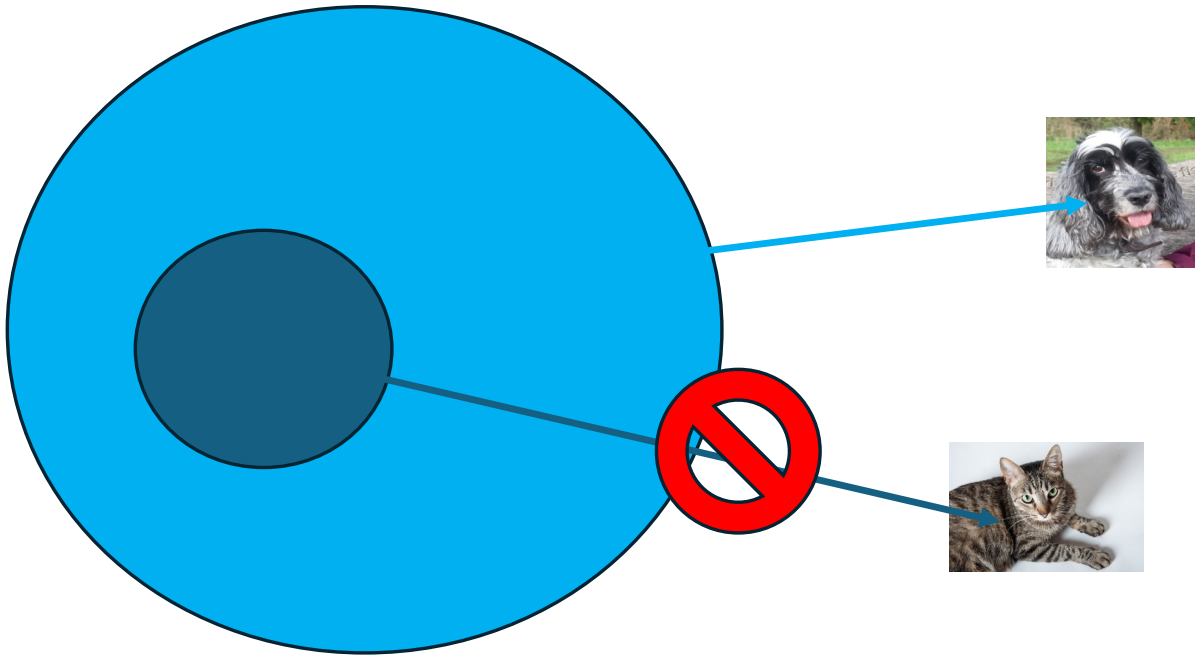
But this data topology cannot be resolved into two points using a smooth Neural ODE



Have to either use a MAP or a non-Lipshitz Neural ODE

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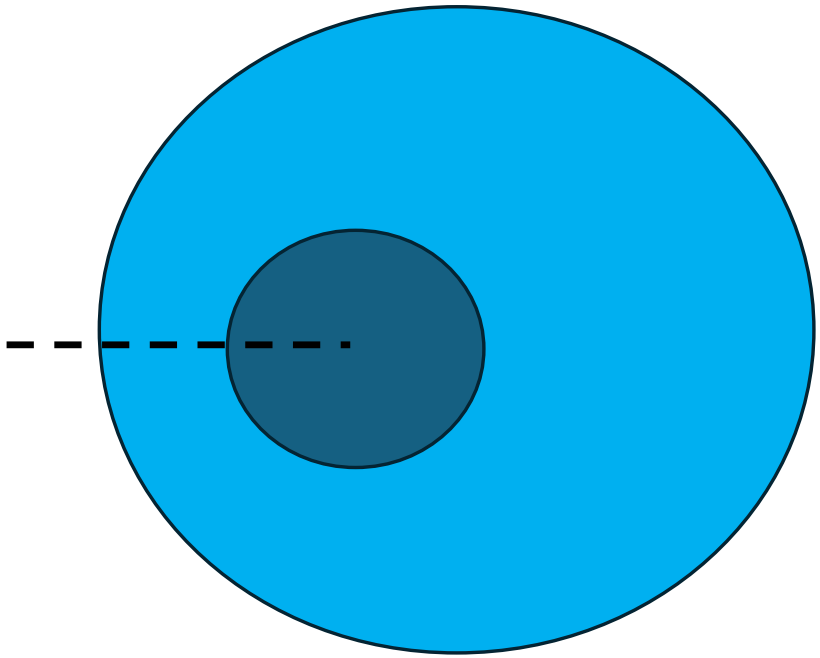
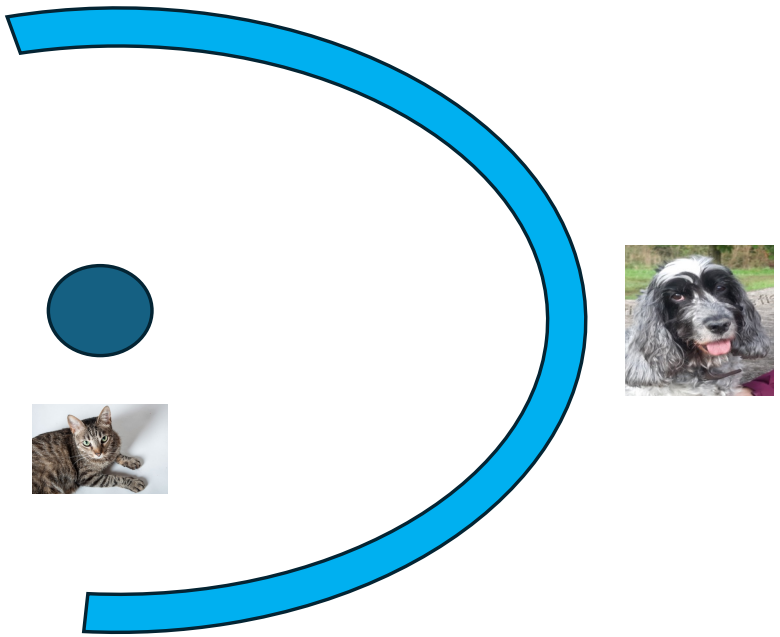
This data topology CAN be resolved using a non-smooth Neural ODE



$$r < 1: \ \frac{dr}{dt} = -r, \quad \frac{d\theta}{dt} = 0, \quad r \geq 1: \ \frac{dr}{dt} = r(r^* - r), \quad \frac{d\theta}{dt} = -\theta.$$

Discontinuous flow breaks the topology and allows data separation



Question: How do we train these systems?

Dynamical systems defined by Neural Nets and learning dynamics from data

Original DS: $$\frac{dx}{dt} = f(x) \qquad x \in R^n$$

Data points: $$y_i = H(x(t_i)) + \epsilon_i, \quad i = 1 \ldots N$$

Train: a NN to approximate this dynamics via:

$$\frac{dz}{dt} = f(z, t, \theta) : \quad \text{f: Neural Net}$$

Also (and confusingly) called a Neural ODE eg. by Matlab

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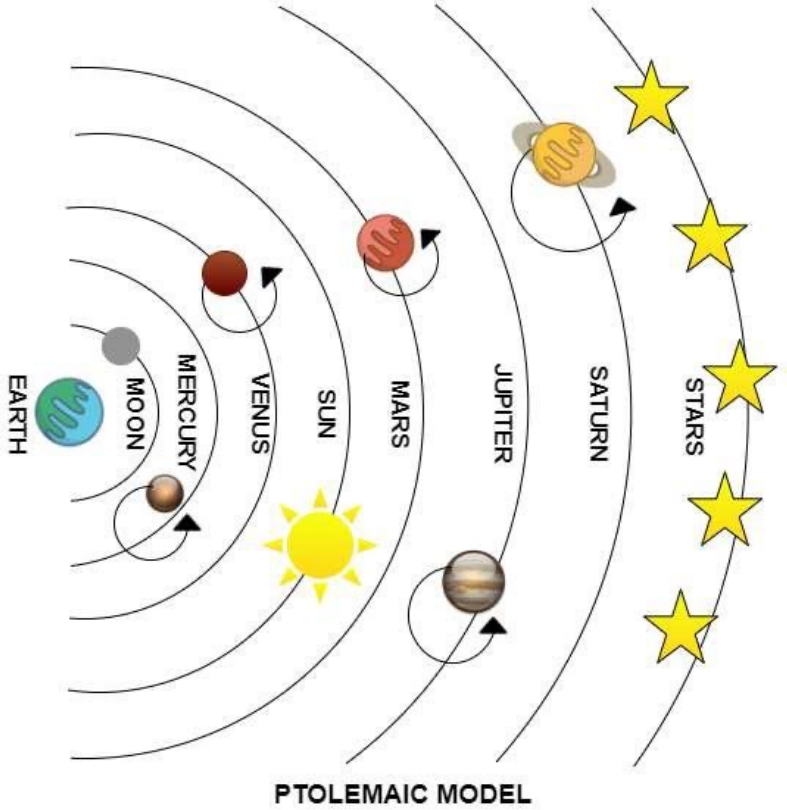
Big literature on these systems



- Ptolemaic model of the solar system
- Standard learning
- Echo State Networks, Reservoir networks
  Especially good for chaotic dynamics
- SINDy approach (Kutze) using a very careful choice of RHS (can even work from video data)

Training such a ‘Neural ODE’. I [From MatLab website]

Example:

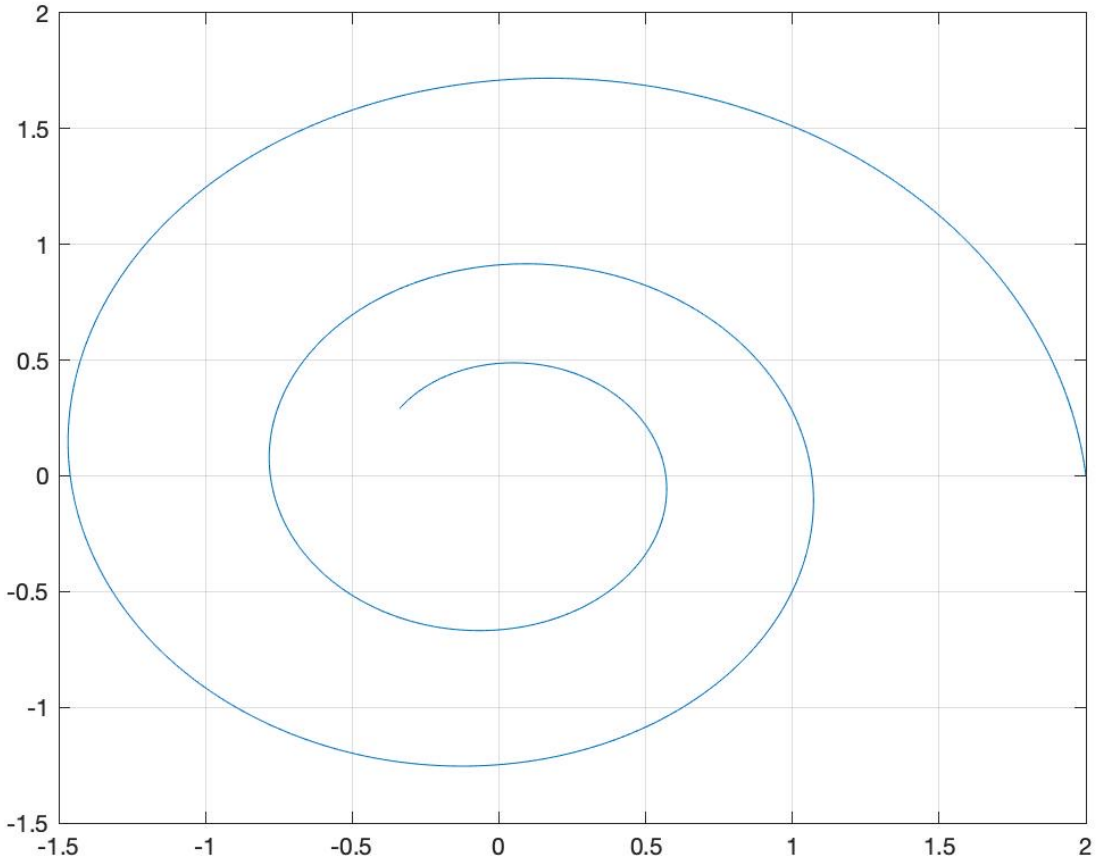
$$\frac{d\mathbf{x}}{dt} = A\mathbf{x}, \quad \mathbf{x} \in R^2$$

$$\mathbf{x}(t) = e^{At}\,\mathbf{x}(0) \equiv B\mathbf{x}(0).$$

Neural ODE: $\dfrac{dz}{dt} = f(z, t, \theta), \quad z(0) = x(0), \quad$ f: Neural Net

Solve: using RK45

Training trajectory starting from: x(0) = [2,0], t = [0,15], 2000 points



$$A = \begin{pmatrix} 0.1 & -1 \\ 1 & -0.1 \end{pmatrix}$$

Define loss: $L(\theta)$

$$L(\theta) = \sum_i |H(z(t_i)) - y_i|^2$$

- Implement NN using 2 layers and tanh activation

$$f(\mathbf{z}, \theta) = W_2 \ \tanh\left(W_1 \ \mathbf{z} + \mathbf{b}_1\right) + \mathbf{b}_2.$$

- Compute gradients directly from the ODE solver using the adjoint method as before
- Optimize using ADAM using first 400 training points

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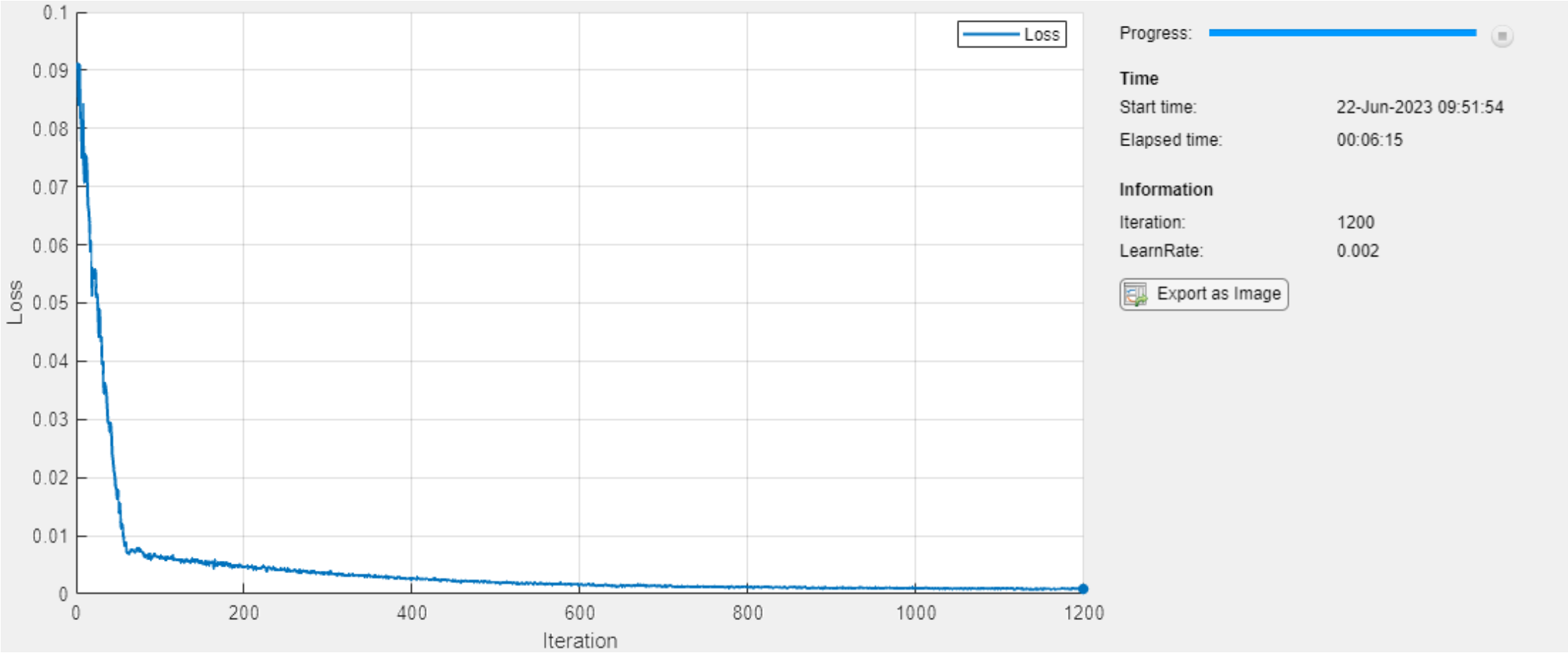
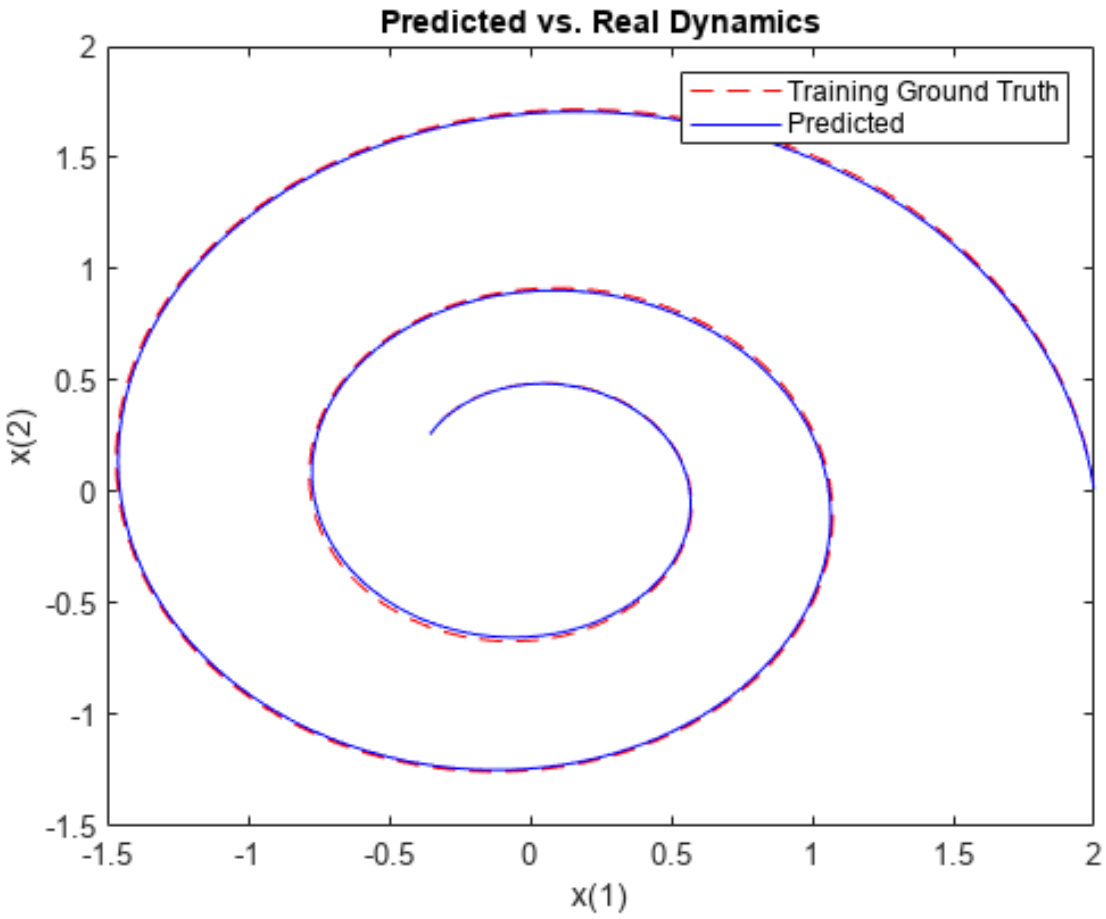
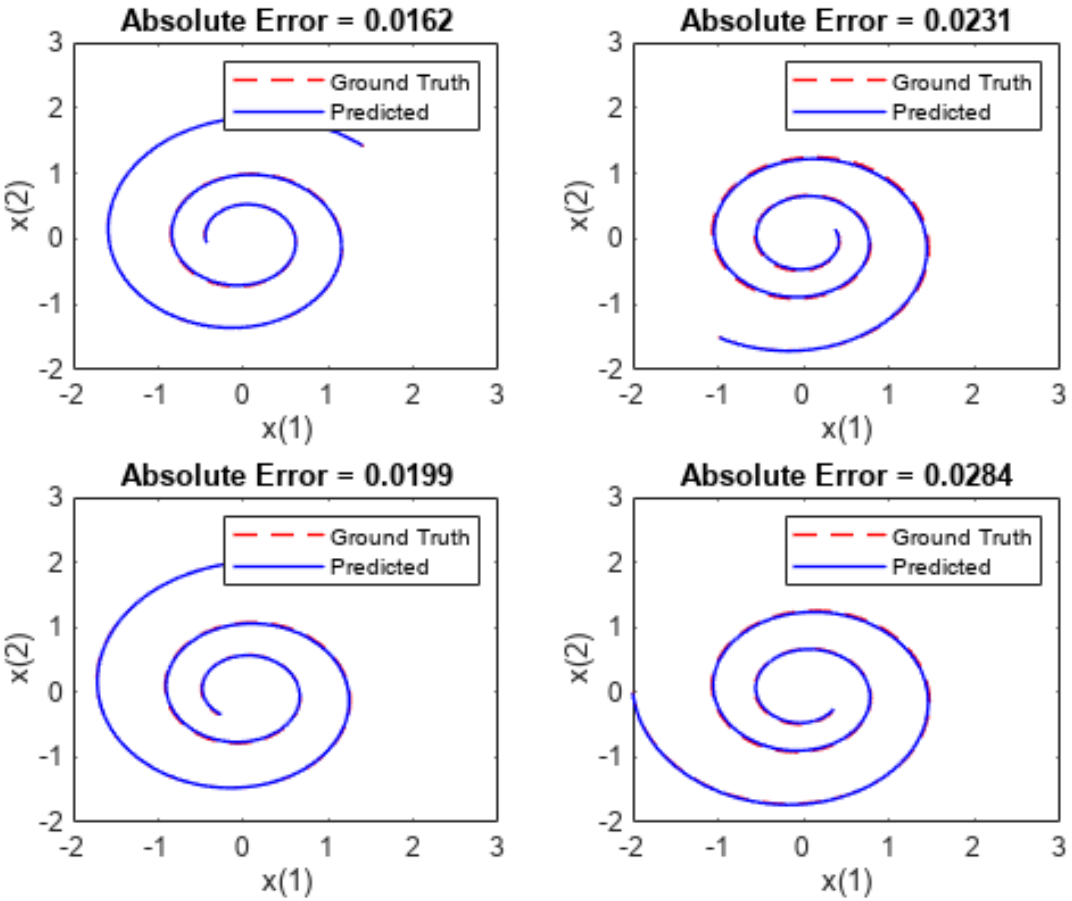
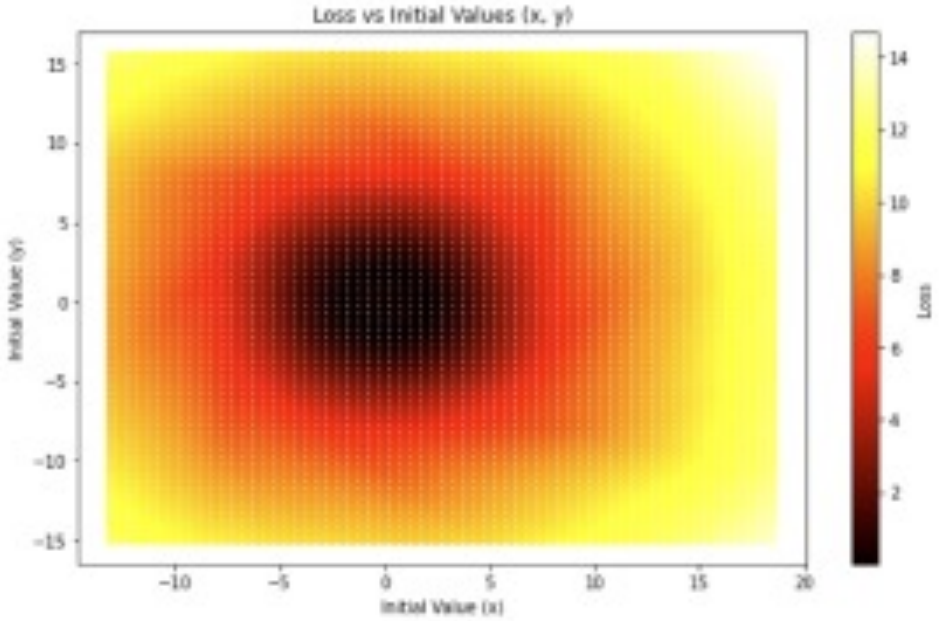

Loss
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
Loss
0
200
400
600
800
1000
1200
Iteration
Progress:
Time
Start time: 22-Jun-2023 09:51:54
Elapsed time: 00:06:15
Information
Iteration: 1200
LearnRate: 0.002
Export as Image

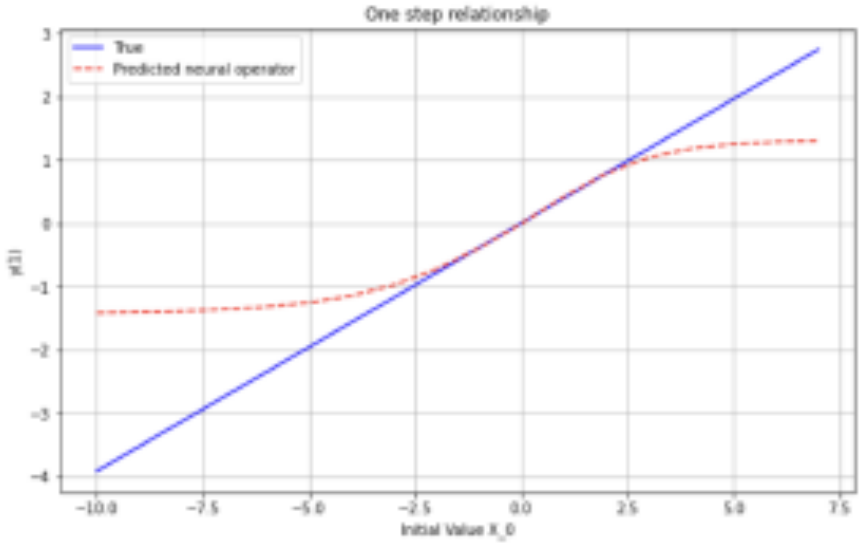

Predicted vs. Real Dynamics
Training Ground Truth
Predicted
x(1)
x(2)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-1.5
-1
-0.5
0
0.5
1
1.5
2

Prediction error is good for initial data close to the training trajectory



Loss increases as we move away from the training trajectory [+Libo Chen]





By way of contrast:

Assume that $$\frac{d\mathbf{z}}{dt} = B\,\mathbf{z}$$

Find matrix B

100 points: $$B = \begin{pmatrix} -0.1001 & -1.0005 \\ 1.0004 & -0.0993 \end{pmatrix}$$

400 points: $$B = \begin{pmatrix} -0.1000 & -1.0005 \\ 1.0007 & -0.1002 \end{pmatrix}$$

2000 points: $$B = \begin{pmatrix} -0.1000 & -1.0005 \\ 1.0005 & -0.1001 \end{pmatrix}$$

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SINDy [Brunton et. al.]

ODE: $$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x})$$

Data: $\mathbf{x}(t_i), \quad \dot{\mathbf{x}}(t_i)$ Plus noise: m measurements

Assume: f(x) can be constructed from a library of known functions

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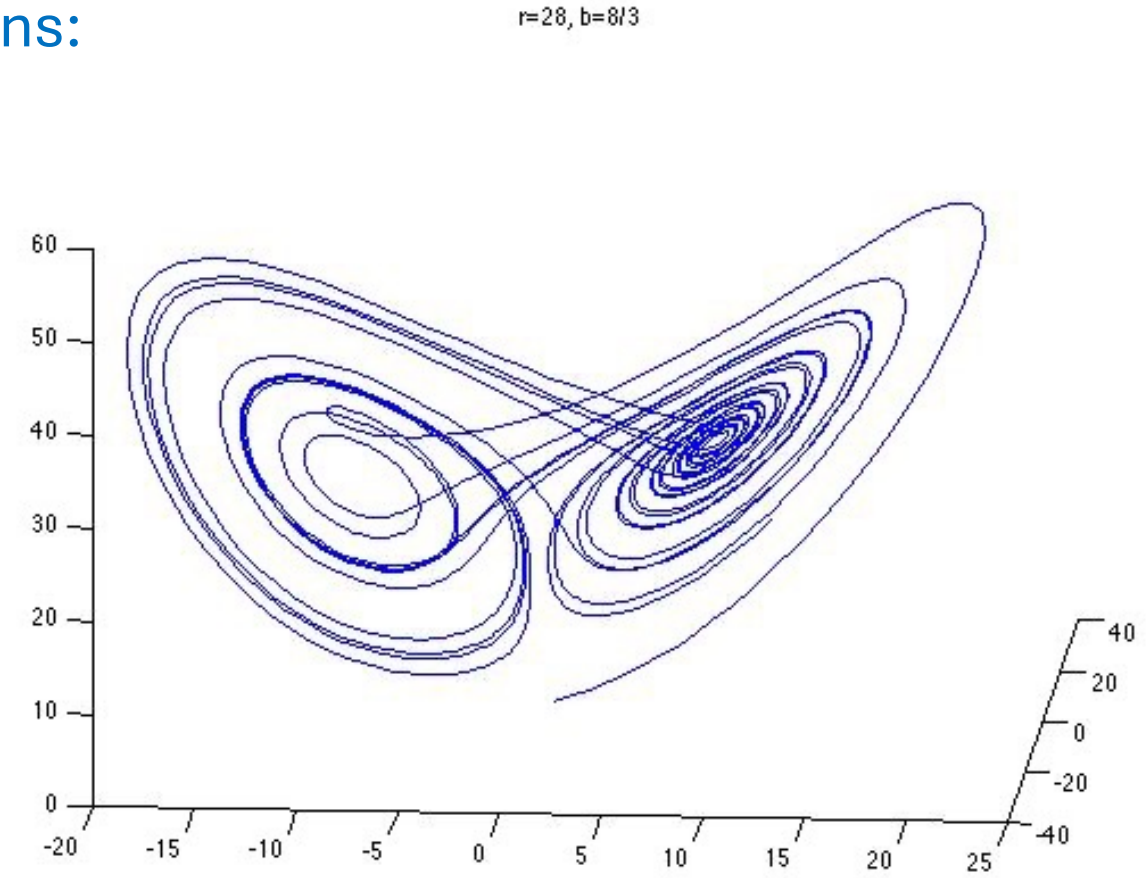
Eg. Lorenz Equations:

$$dx/dt = \sigma(y - x),$$
$$dy/dt = x(\rho - z) - y,$$
$$dz/dt = xy - \beta z.$$



Library: $\Theta(\mathbf{x}) = \left[\mathbf{1} \mid \mathbf{x} \mid \mathbf{x}^{P_2} \mid \mathbf{x}^{P_3} \mid \sin(\mathbf{x}) \mid \cos(\mathbf{x}) \mid \ldots\right]$

Size. m x p m >> p

Coefficients (sparse vectors): $\Xi = \left[\xi_1 \; \xi_2 \; \ldots \; \xi_n\right]$

Seek a SPARSE approximation of the form:

$$\dot{\mathbf{x}} = \Theta(\mathbf{x})\, \Xi$$

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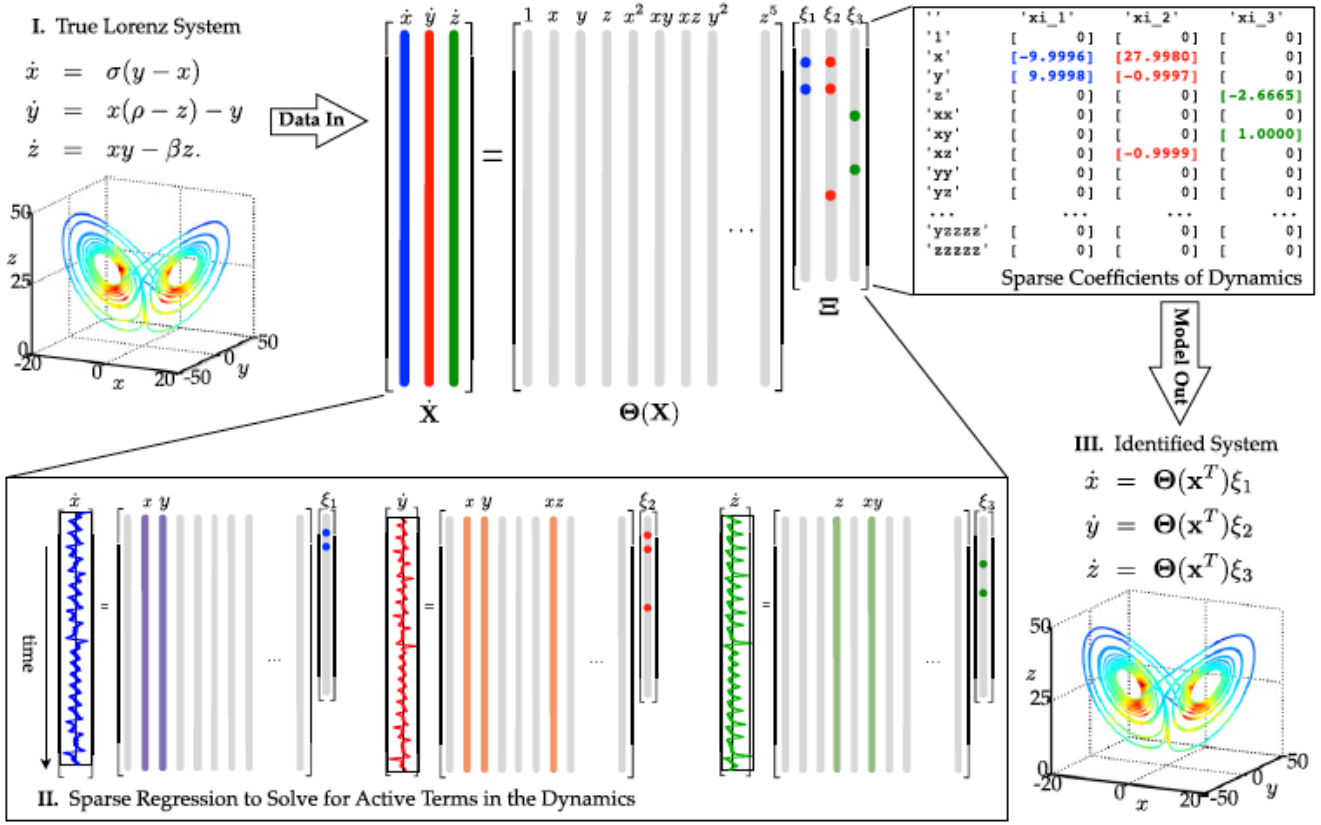
Aim: Find best set Ξ to fit to (filtered, noisy) data

Possibly with numerically estimated derivatives



From Brunton et. el.

Possible dynamics of Neural ODEs

$$\frac{dx}{dt} = f(x, \theta)$$

f(.) output of a feed-forward Neural Network

f(.) Can be piecewise smooth, continuous or even discontinuous

Non-smooth nature of the dynamics places a significant constraint on the possible dynamics of the neural ODE, and helps understand what dynamics might be possible

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For example, NN naturally lead to:

Filippov Flows

$$f(x,\theta) = f_i(x,\theta), \quad x \in S_i,$$

$$\bar{S}_i \cap \bar{S}_j \equiv \Sigma_{ij}$$

Smooth flow in sets S_i

Transitions across boundaries Σ_{ij}

Possible sliding along Σ_{ij} if f is discontinuous across the boundary

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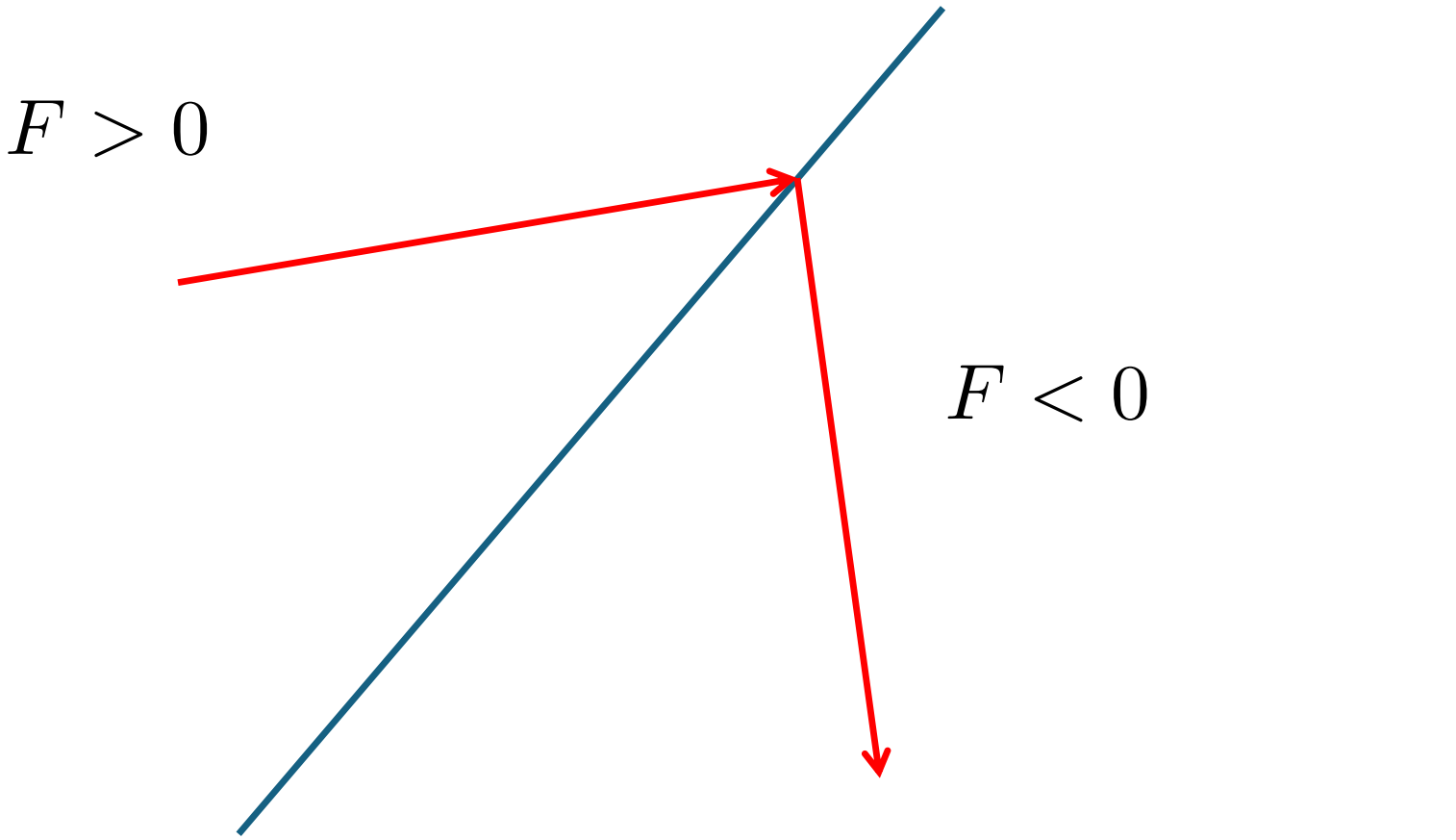
Filippov dynamical system without sliding

$$\Sigma = \{\mathbf{X} : F(\mathbf{X}) = 0\}$$



Typical ‘transverse’ intersection

Features of non-smooth flows

- Discontinuity induced bifurcations [di Bernardo et. al.]
  - Border collision bifurcations when a fixed point intersects Σ_{ij}
  - Non-smooth folds
  - Grazing bifurcations when a flow has a non-transverse intersection with Σ_{ij}
- Period-adding and period-incrementing routes to chaos
- Robust Chaotic Behaviour is very common due to the stretching of phase space by the discontinuities/non-smooth effects [Banergee, Hogan]. Sensitivity to initial conditions and parameters.

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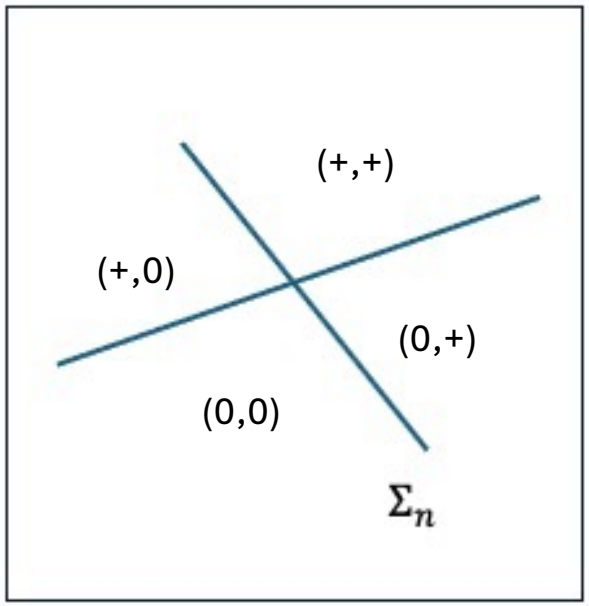
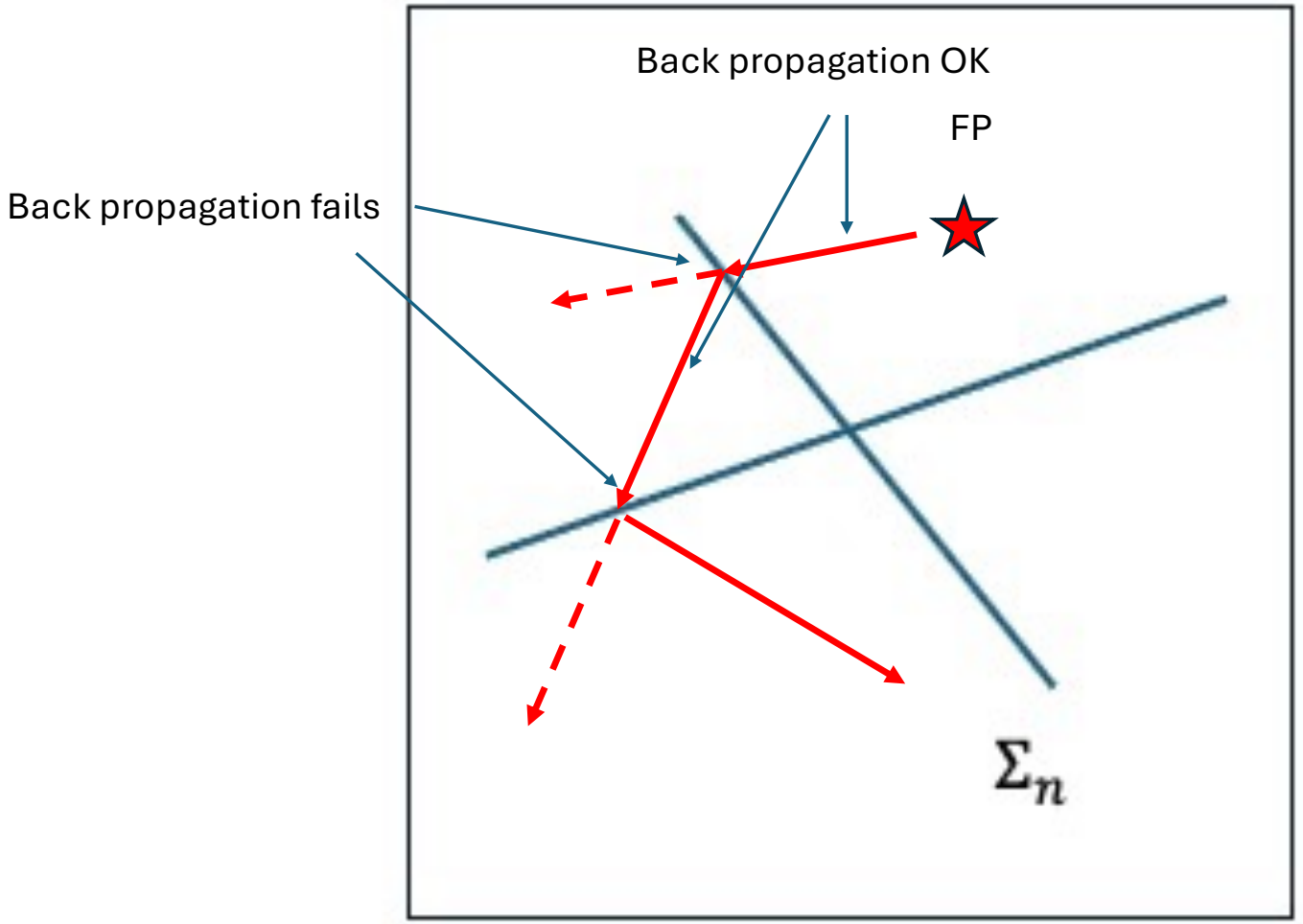
Example: Fixed point, Limit Cycle, and Chaotic Dynamics in ReLU type ODEs

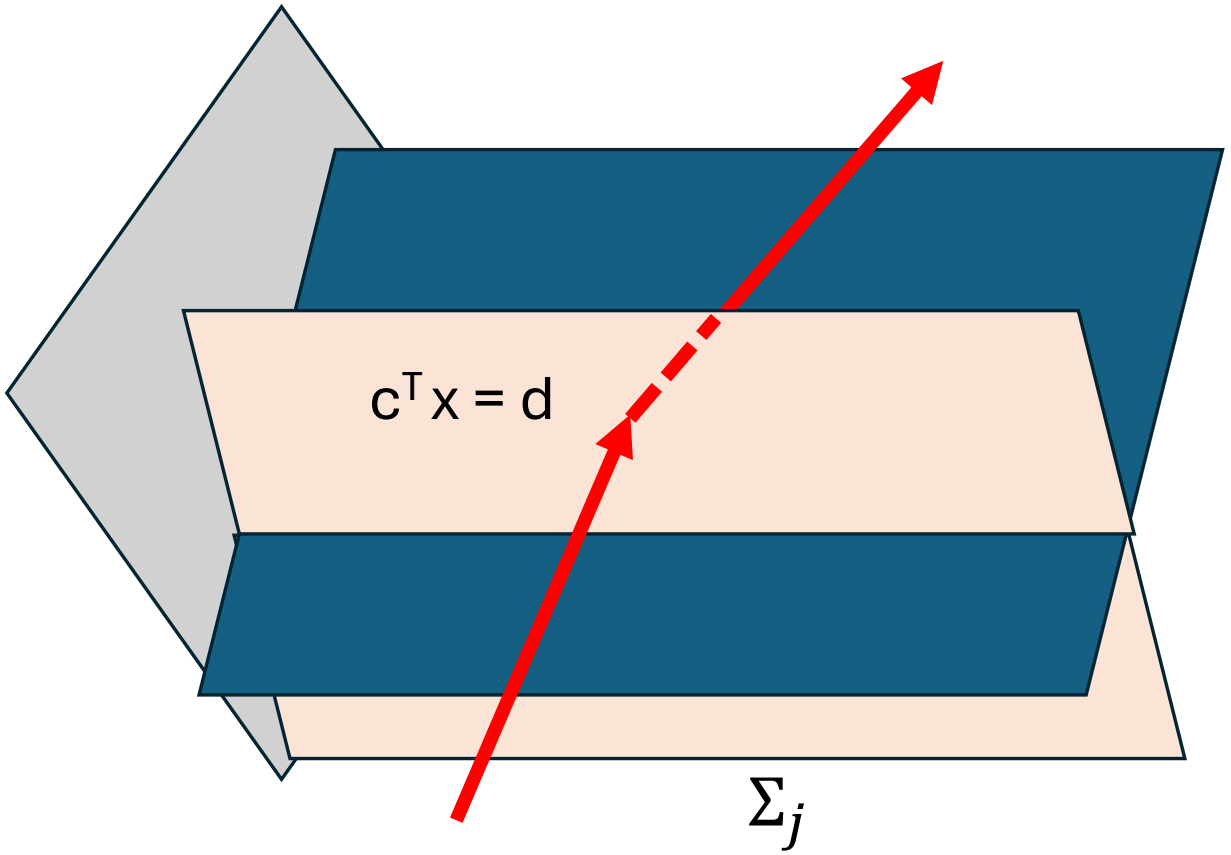
$$\frac{dx}{dt} = A_1 x + b_1 + ReLU(A_2 x + b_2)$$



Evolution of a fixed point. (2-dimensions)



Local behaviour (n – dimensions) when back propagation fails



General case: Normal form at the transition

All ReLU type dynamics can be expressed locally close to the switch manifold as:

$$\frac{dx}{dt} = A_1 x + \mu\, b \quad if \quad c^T x < 0,$$
$$\frac{dx}{dt} = A_2 x + \mu\, b \quad if \quad c^T x \geq 0.$$

Possible scenarios:

- FP → FP
- FP + FP → ∅
- FP → Limit cycle
- FP → Chaos

Can classify many of the transitions in terms of the structure of A_i and b.

[Freire], [Carmona]

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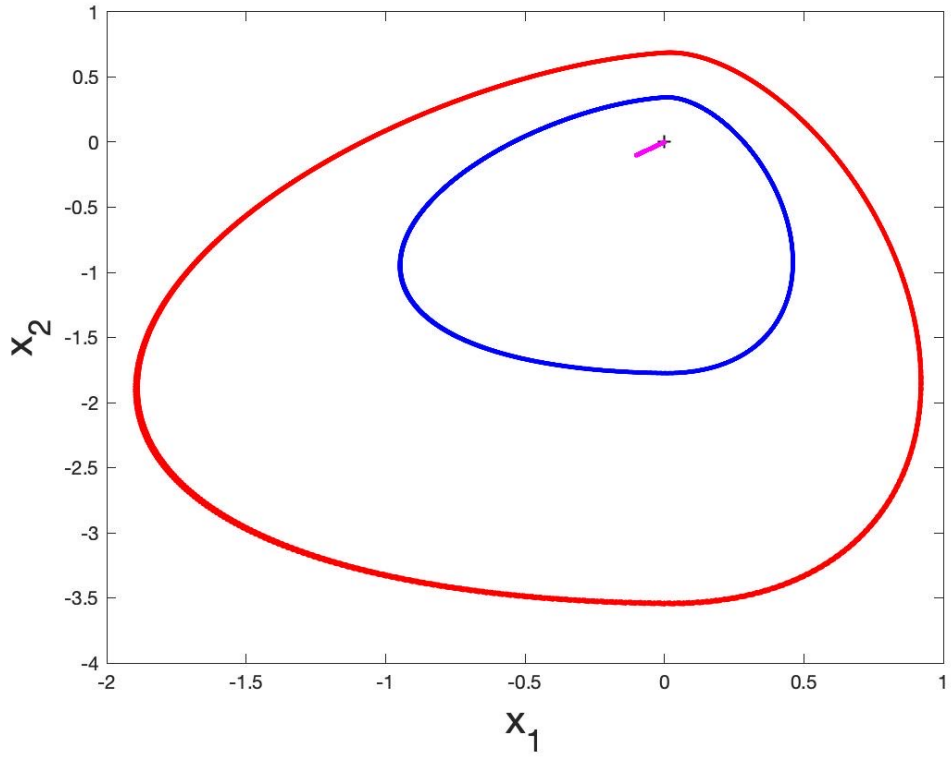
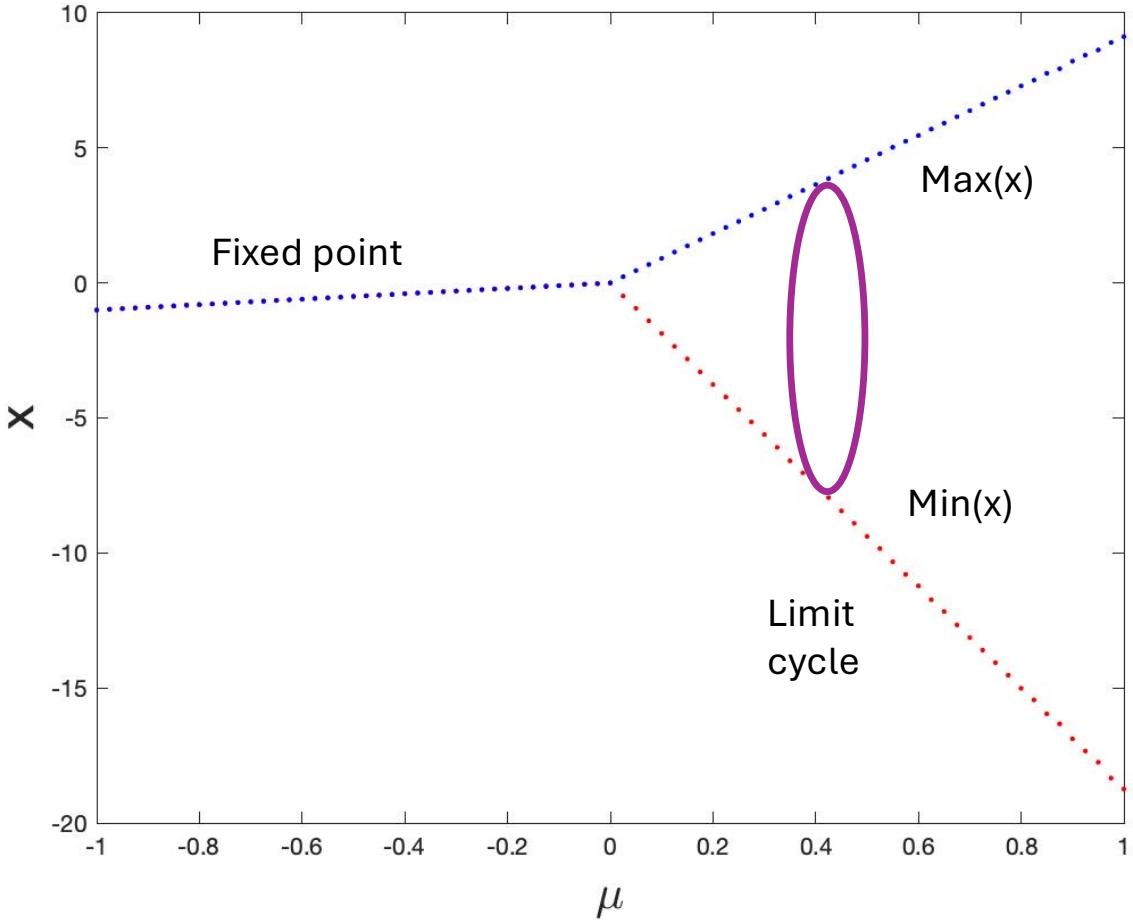
Example: FP → Limit Cycle

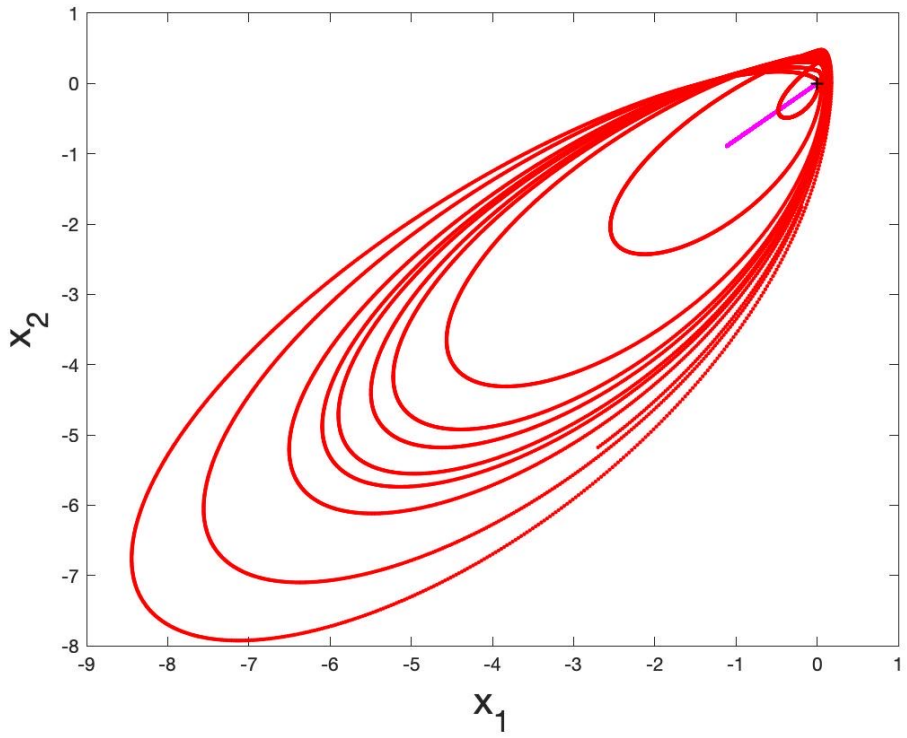
$$A_1 = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 2 & 1 \\ -5 & 0 \end{pmatrix}, \quad b = (0\ 1)^T, \quad c = (1\ 0)^T$$

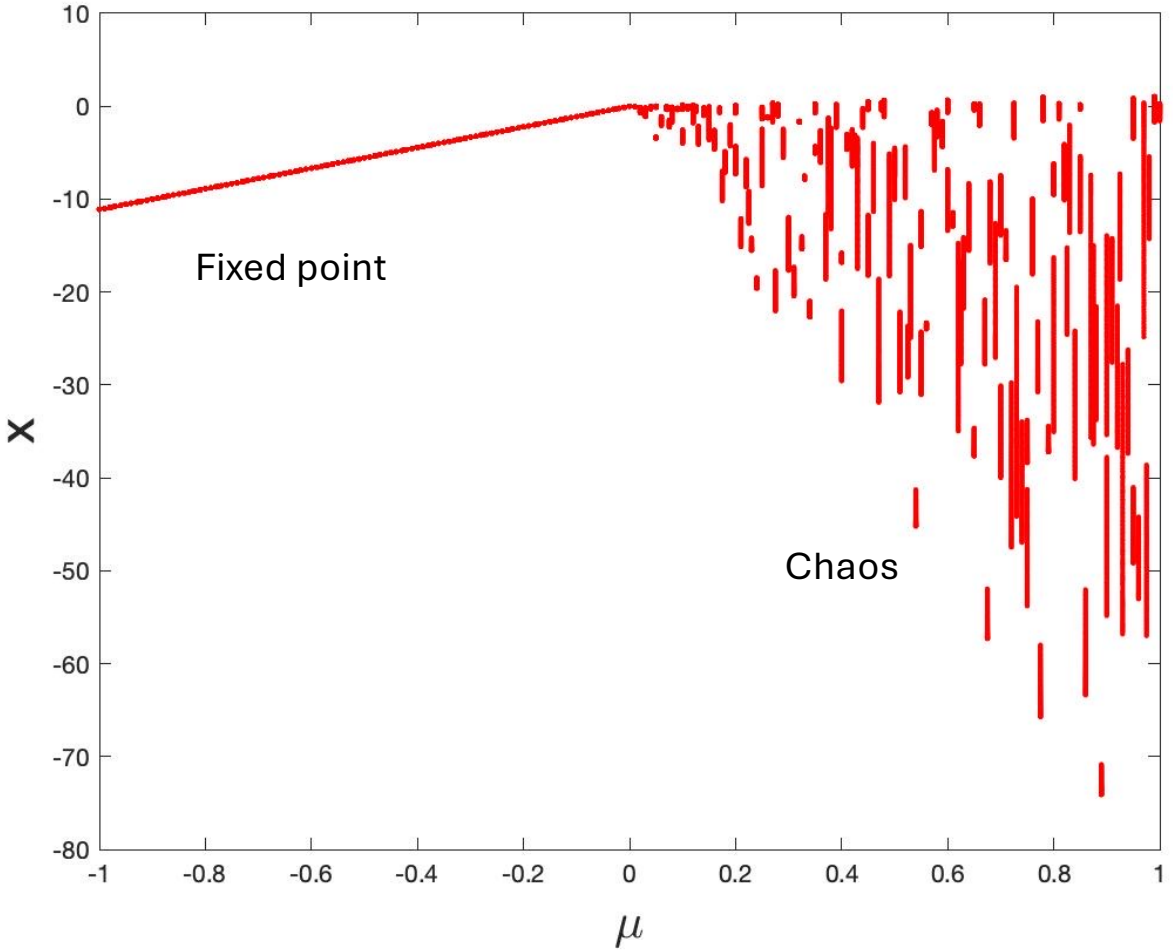



Fixed point
Max(x)
Min(x)
Limit
cycle
x
μ
10
5
0
-5
-10
-15
-20
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

Example 2: FP → Chaos

$$A_1 = \begin{pmatrix} 0.8 & 1 & 0 \\ 0.57 & 0 & 1 \\ -0.09 & 0 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0.1 & 1 & 0 \\ -0.2 & 0 & 1 \\ -60 & 0 & 0 \end{pmatrix}, \quad b = (0\ 0\ 1)^T, \quad c = (1\ 0\ 0)^T$$




Fixed point
Chaos
x
μ
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

Conclusions

Neural ODEs are effective for

- Describing the flow through a NN
- Learning dynamics from data
- They inherently non smooth (or close to non smooth)
- They work best when informed by the physics