Jacobian norm regularisation and conditioning in neural ordinary differential equations

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06 December 2022

What to expect

Overview of neural ordinary differential equations (ODEs)

- learnable input-output mapping defined as the solution to an ODE

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Neural ODE challenges and Jacobian regularisation

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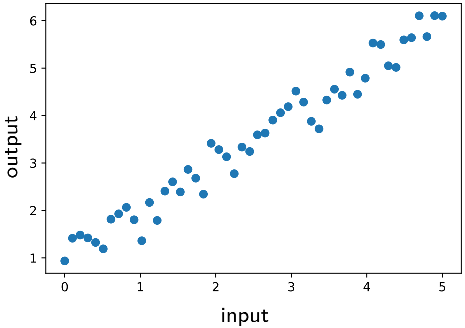
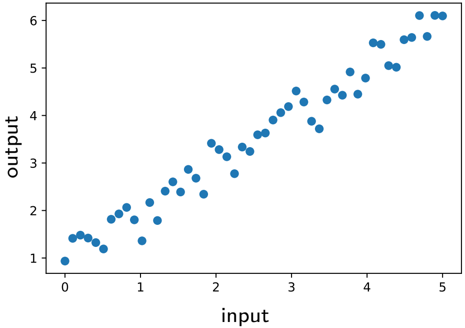
Review selected results

Learnable input-output mapping



Learnable input-output mapping



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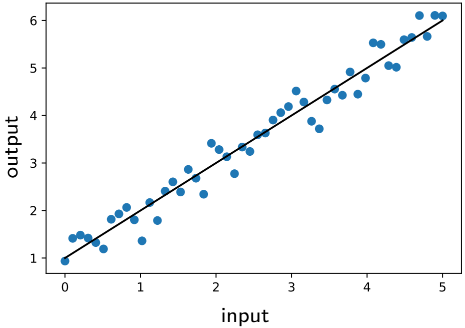
$$f(x) = wx + b$$

Learnable input-output mapping



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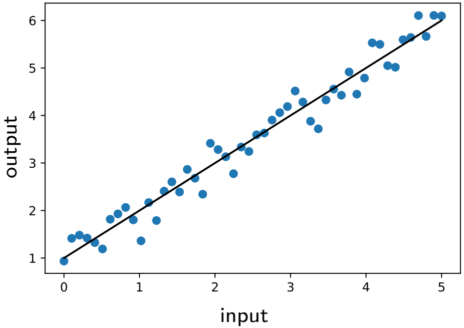

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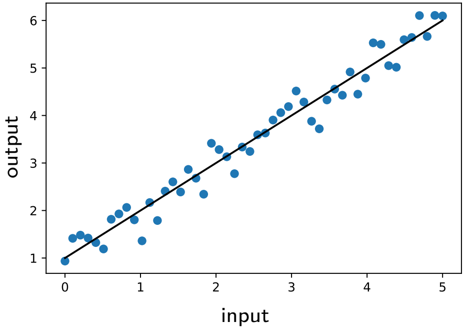

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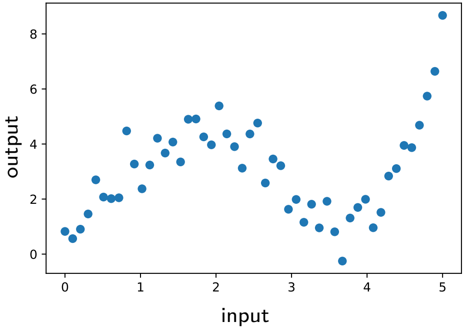
Regularisation adds a penalty to the objective.

- faster convergence, better generalisation

Learnable input-output mapping: neural networks



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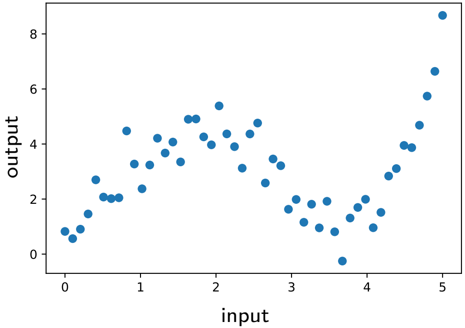

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$$f(x) = f^n \circ f^{n-1} \circ \cdots \circ f^1(x)$$

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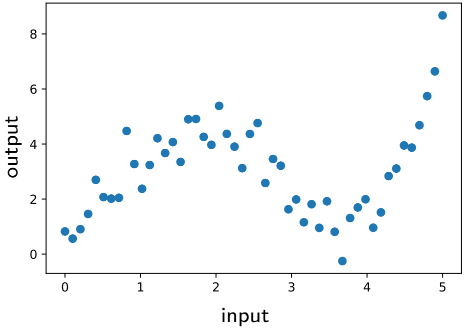

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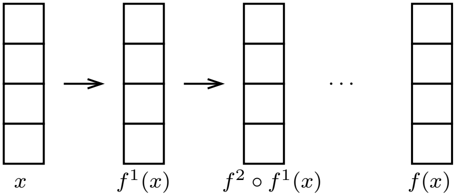

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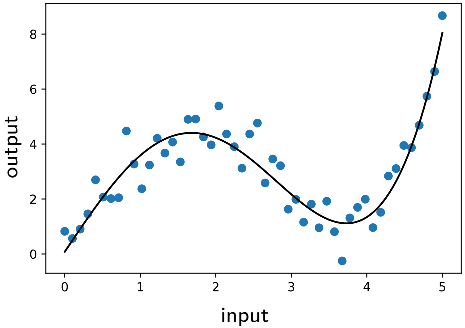

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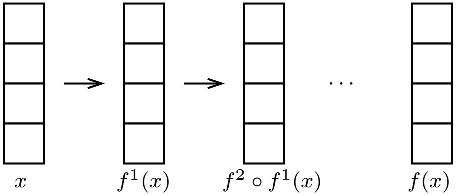

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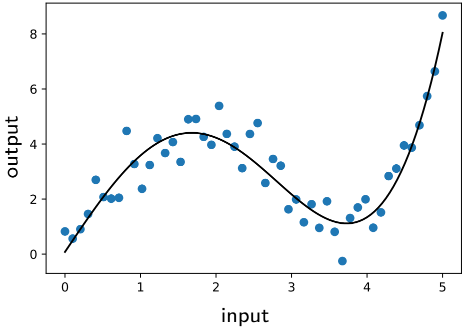

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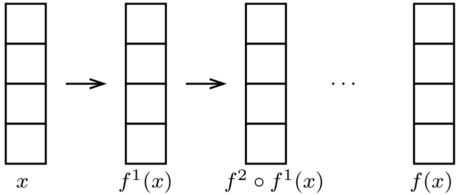

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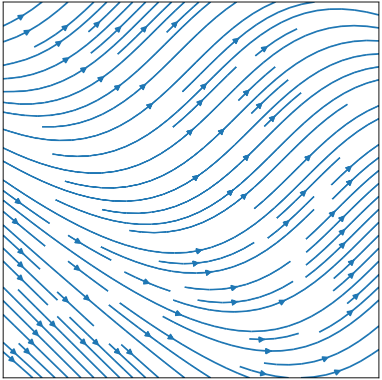
Neural ordinary differential equations

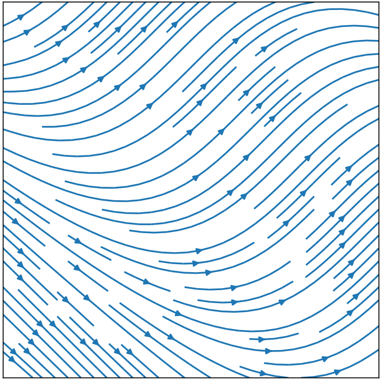


A vector $\boldsymbol{h}(t)$ follows the dynamics f:

$$\frac{d\boldsymbol{h}(t)}{dt} = f(\boldsymbol{h}(t), t)$$

Neural ordinary differential equations

$\boldsymbol{h}(t_0)$



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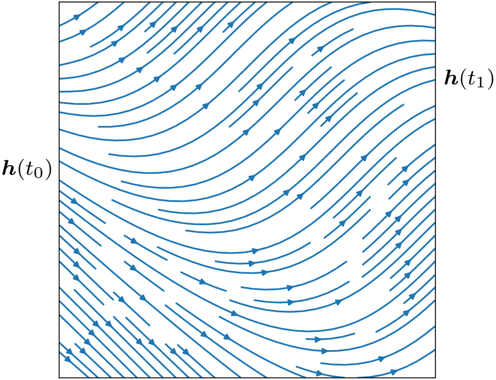

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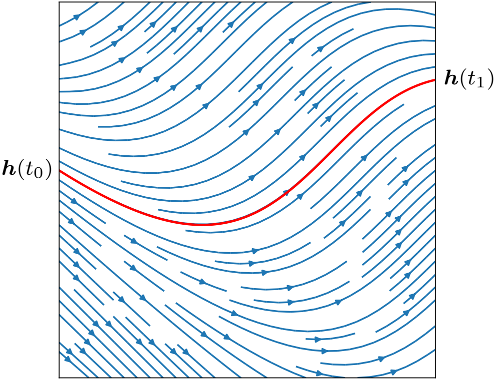

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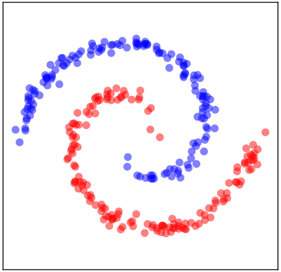
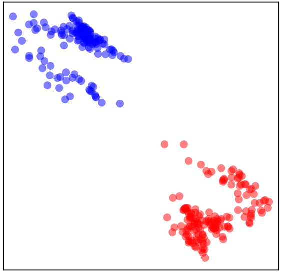
An example: binary classification



input

use a neural network
as the function



output

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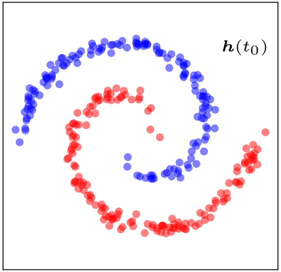

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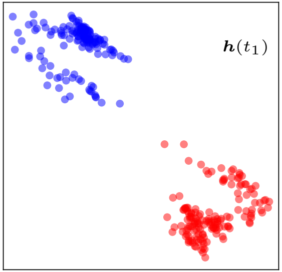

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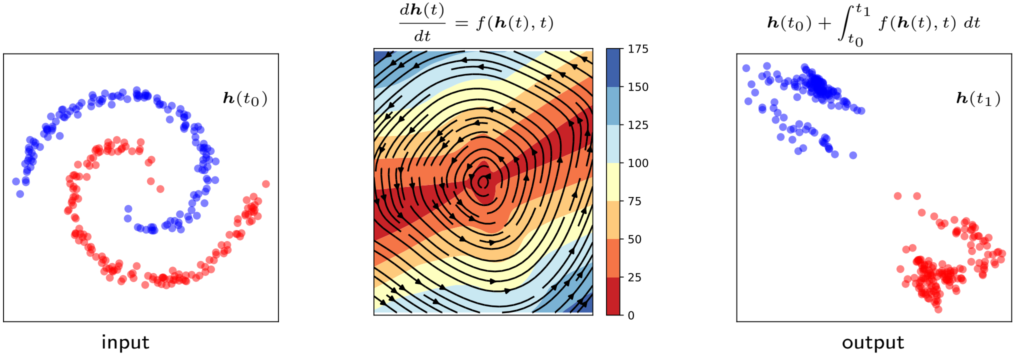

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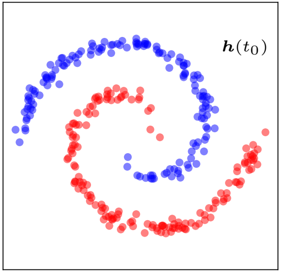
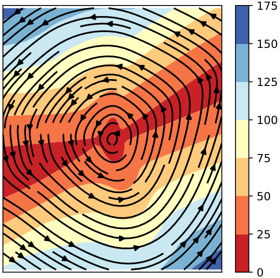


input

$$\frac{d\boldsymbol{h}(t)}{dt} = f(\boldsymbol{h}(t), t)$$



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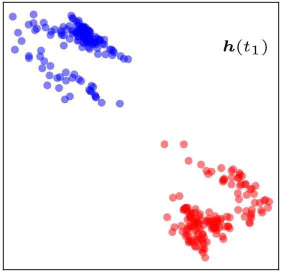

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More generally useful for

An example: binary classification

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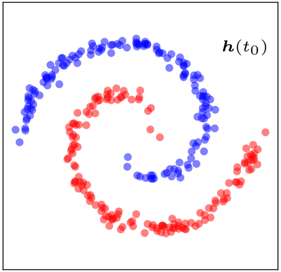

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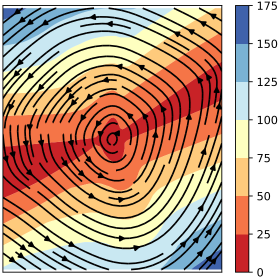

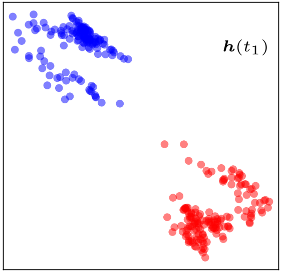

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More generally useful for

1. Modelling data from continuous-time systems

dynamical systems, time-series

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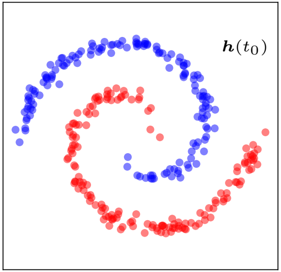

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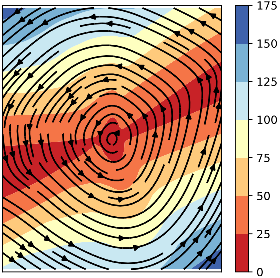

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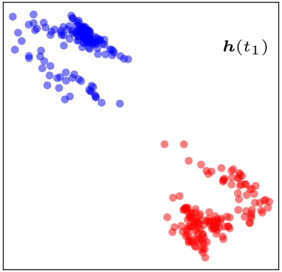

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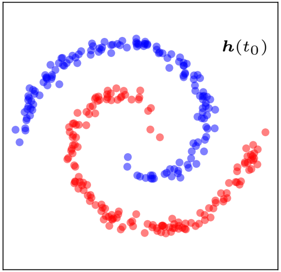
More generally useful for

1. Modelling data from continuous-time systems — dynamical systems, time-series
2. Continuous normalising flows for density estimation

An example: binary classification



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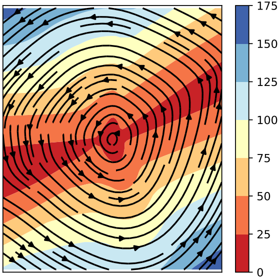

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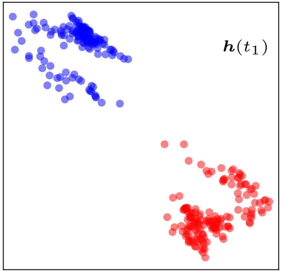

output

We care about

An example: binary classification

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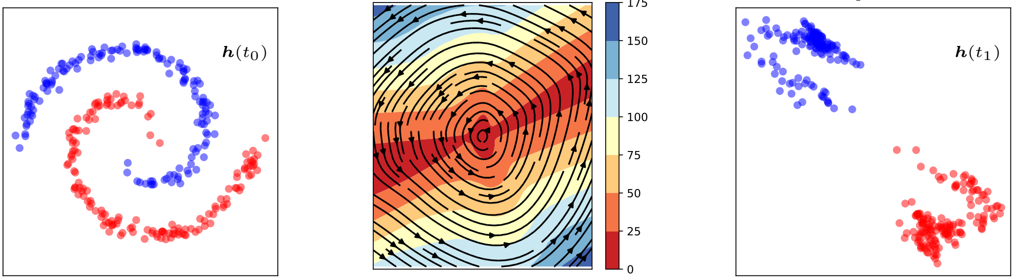


input

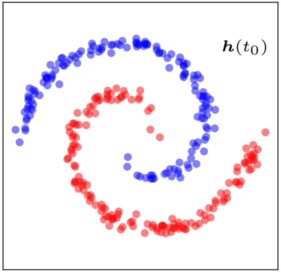
output

We care about

1. Generalisation and robustness to input perturbations

in high dimensions

An example: binary classification



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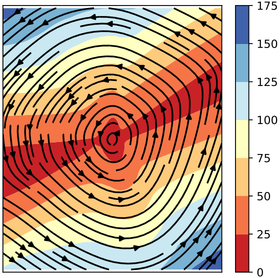

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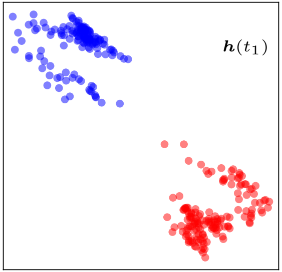

output

We care about

1. Generalisation and robustness to input perturbations
2. Computational efficiency

in high dimensions

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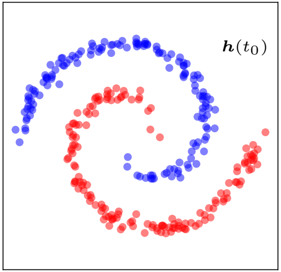

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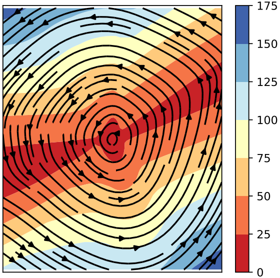

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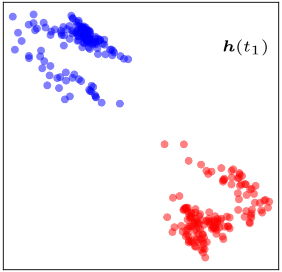

output

We care about

1. Generalisation and robustness to input perturbations — in high dimensions
2. Computational efficiency

How should we regularise our objective function when training neural ODEs?

The problem: rising number of function evaluations (NFE)

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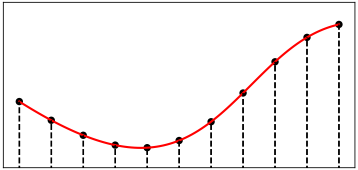

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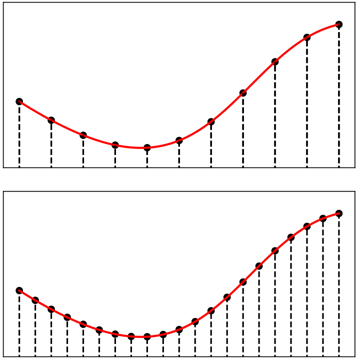

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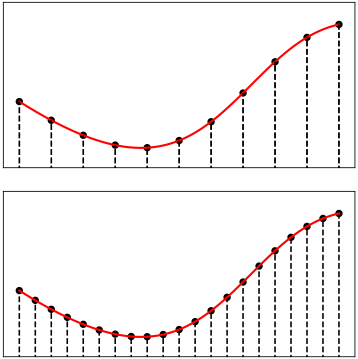

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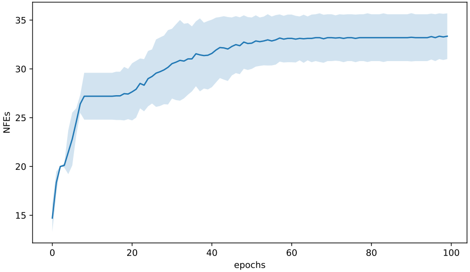

NFE rises during training

Comments on conditioning

"poorly conditioned dynamics will lead to difficulties during numerical integration"

Finlay et al. How to train your neural ODE: the world of Jacobian and kinetic regularization, 2020.

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"flows that need to stretch and squeeze the input space in such a way are likely to lead to ill-posed ODE problems that are numerically expensive to solve"

Dupont et al. Augmented Neural ODEs, 2019.

Jacobian norm regularisation

If $\boldsymbol{h}(t) = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$, and $f(\boldsymbol{h}(t), t) = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$, then $\boldsymbol{J} = \begin{bmatrix} \frac{\partial f_1}{\partial h_1} & \frac{\partial f_1}{\partial h_2} \\ \frac{\partial f_2}{\partial h_1} & \frac{\partial f_2}{\partial h_2} \end{bmatrix}$

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Frobenius: neural ODE

Jacobian norm regularisation

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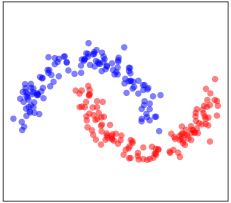
Jacobian norm regularisation



Binary classification

Intertwining moons dataset

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Frobenius: neural ODE

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spectral: neural network

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condition number: our work

NFE reduction

Frobenius, spectral, and condition number regularisation reduce NFE.

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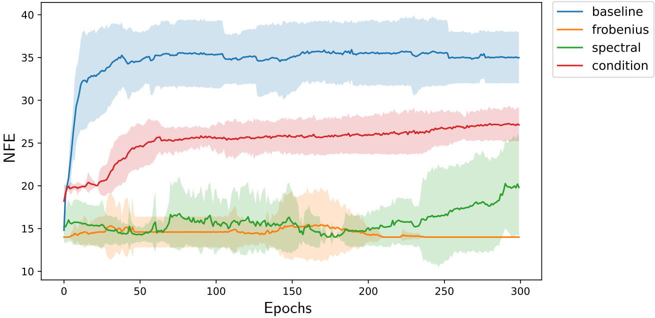

Solid curves and shaded regions indicate mean and standard deviation over 10 runs.

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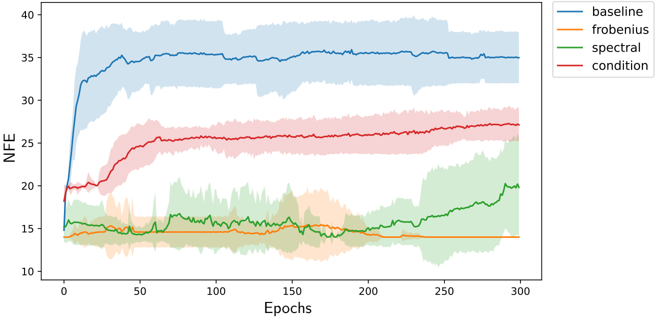

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Good! But at what cost?

Performance and robustness

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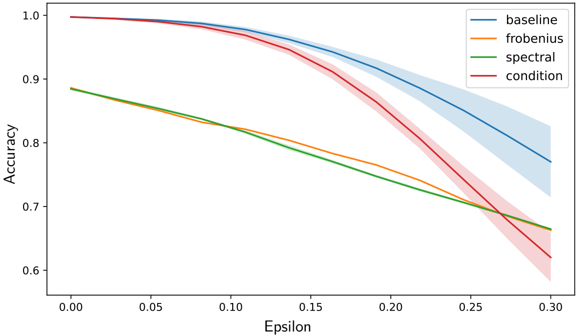

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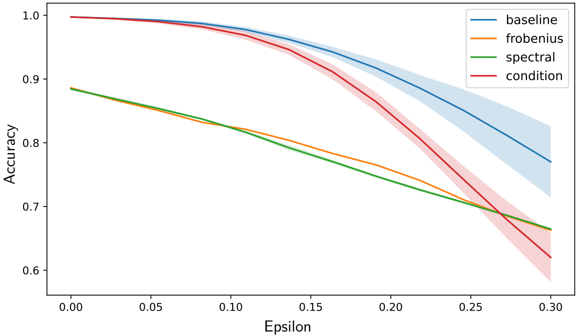

Jacobian norm regularisation leads to increased distance to decision boundary.

Effect on conditioning

Condition number an explanation for robustness?

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Intertwining moons	
Regularisation	Condition number
None	5.3 ± 3.5
Frobenius	27.3 ± 34.1
Spectral	45.9 ± 70.6
Condition number	6.1 ± 5.2

Conclusion

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Ongoing work:

1. Efficient condition number estimation.
2. Characterise conditions for rising NFE (stiffness?).
3. Other ways to parameterise the ODE or solution?